

Award DFEG02-03ER15476, The Reactivity and Structural Dynamics of Supported Metal Nanoclusters Using Electron Microscopy, in-situ X-Ray Spectroscopy, Electronic Structure Theories, and Molecular Dynamics Simulations

PI: Ralph Nuzzo. Co-PIs: Anatoly Frenkel, Duane Johnson, Judith Yang, John Rehr, Eric Stach

Accomplishments (2003-2019)

Our work conducted in the 2003-2019 grant periods has yielded several forms of progress. Foremost in this regard is the extensive progress that has been made within the collaborative efforts of the PIs to establish a validated toolset for the characterization of the nanoscale materials that are found ubiquitously in heterogeneous catalytic processes. For our work, the applications of XAS, electron microscopy and first principles simulations, as well as the development of operando techniques for studies of catalytic materials have been particularly fruitful, and have allowed us to pose and answer important fundamental questions in nanoscale materials science of direct relevance in catalysis. We list our main accomplishments below, in reverse chronological order, followed by the complete publication list acknowledging this award.

1. We have developed, tested, and utilized a new method of correlative multi-modal (spectroscopy and imaging) analysis of single atom catalysts, a building block of a multi-component catalytic system. This method exploits a combination of XAS (XANES and EXAFS), STEM, AP-XPS and Resonant Inelastic X-ray Scattering (RIXS), and enables operando characterizations of catalysts as they evolve from single atom to metallic speciations in real working conditions.
2. We utilized the data science methods to enable quantitative analysis of XANES to reveal structural information currently available through the multiple scattering (MS) EXAFS analyses.
3. We illustrated the utility of the advanced synchrotron spectroscopies (high energy resolution fluorescence detection and RIXS) as tools for the structural characterization of catalysts when joined with supervised machine learning (SML) -assisted methods of data analysis.
4. We have developed, tested, and utilized a new method of correlative multi-modal (spectroscopy and imaging) analysis of working nanocatalysts that highlighted the complex structural dynamics of supported Pt and Pd catalysts. This method exploits a microfabricated catalytic reactor compatible with both probes.
5. We utilized the high-energy resolution absorption (HERFD XANES) and emission (RIXS) spectroscopies to highlight the role of intra-catalyst heterogeneity of atoms and charges, and their dynamic rearrangements during catalytically relevant conditions.
6. We highlighted the role of first principle simulations (DFT/MD-based) theory in obtaining the links that exist between multiple components of a catalytic system (e.g. the precise atomic structure of a catalytic cluster, of a supporting oxide, and the bonding patterns of adsorbates) and the properties that are exhibited under reaction conditions.
7. We have broadly demonstrated the utility of advanced XAS spectroscopies as a means through which the complex microscopic attributes of electronic charge distributions in a catalyst, and the mechanisms through which environmental conditions (e.g. temperature and pressure) modify them, can be understood—and further developing new theoretical frameworks for their analysis. These studies established the importance of high-energy resolution in the spectroscopic measurements in supporting advances made in theoretical modeling.
8. We developed quantitative methods of electron microscopy (e.g. QSTEM, for shape determination in supported metal catalysts and EELS, for studies of catalyst-support interface) that are complementary in nature to XAS-based measurements and provide important single-cluster-specific constraints to theory.
9. We have applied XAS spectroscopies (XANES and EXAFS) *in operando*, to investigate many features relevant to catalytic properties, work that includes investigation of temperature and

pressure dependent bonding dynamics of supported metal-cluster catalysts to adsorbates and an extensive preliminary *operando* investigation of surprising structural complexities and reconstructions of the catalysts evidenced in the hydrogenation of ethylene.

10. We demonstrated that the structural dynamics of small metallic clusters is quite complex. It is characterized by multiple length and time scales, heterogeneity of crystalline orders and morphologies, and non-bulklike electronic properties. Small clusters also embed significant strains in their interatomic bonding that are strongly responsive to the *in-operando* conditions under which the catalytic system operates.
11. Our experimental efforts have definitively established the essential mesoscopic nature of dynamics in such systems, ones that lead to complex impacts on equilibrium structure and its composition, temperature, and adsorbate-dependent evolution. This work has clarified the strong size-dependent scaling of equilibrium structure in such systems—a sensitivity that challenges long adopted (but inadequate) models of metal cluster structure in supported catalysts—and the deterministic role that precise chemical and dynamical details of the metal-support interactions play in mediating them. Taken together the work has opened a new window on how non-equilibrium, e.g., fluxional, librational and/or diffusive behaviors contribute critically to materials properties in supported catalysts, with suggestions as to how those dynamic properties in turn might serve to influence catalytic function (i.e., reactivity).

Publications (2003-2019)

Papers exclusively funded by the grant and jointly funded by the DOE award and other grants with leading intellectual contribution from the DOE grant

1. Y. Li, M. Kottwitz, J. Vincent, Z. Liu, L. Zhang, J. Huang, S. D. Senanayake, P. A. Crozier, R. G. Nuzzo, A. I. Frenkel
Dynamic structure of active sites in ceria – supported Pt catalysts for the Water Gas Shift reaction
Nature Commun. **12**, 914 (2021)
2. L. Kang, X. Y. Liu, A. Wang, L. Li, Y. Ren, X. Li, X. Pan, Y. Li, X. Zong, H. Liu, A. I. Frenkel, T. Zhang
Photo-thermo catalytic oxidation over TiO₂-WO₃ supported platinum catalyst
Angew. Chem. Int. Ed. **132**, 13009-13016 (2020)
3. Y. Liu, N. Marcella, J. Timoshenko, A. Halder, B. Yang, L. Kolipaka, M. J. Pellin, S. Seifert, S. Vajda, P. Liu, A. I. Frenkel
Mapping XANES spectra on structural descriptors of copper oxide clusters using supervised machine learning
J. Chem. Phys. **151**, 164201 (2019)
4. X. Chen, D. A. Henckel, U. Nwabara, Y. Li, A. I. Frenkel, T. Fister, P. J. A. Kenis, A. A. Gewirth
Controlling speciation during CO₂ reduction on Cu-alloy electrodes
ACS Catalysis **10**, 672-682 (2020)
5. J. Timoshenko, A. I. Frenkel
“Inverting” X-ray Absorption Spectra of catalysts by machine learning in search for activity descriptors
ACS Catalysis (Perspective) **9**, 10192-10211 (2019)
6. Liu, D.; Li, Y.; Kottwitz, M.; Yan, B.; Yao, S.; Gamalski, A.; Grolimund, D.; Safonova, O. V.; Nachtegaal, M.; Chen, J. G.; Stach, E. A.; Nuzzo, R. G.; Frenkel, A. I.
Identifying dynamic structural changes of active sites in Pt-Ni bimetallic catalysts using multimodal approaches ACS Catalysis **8**, 4120-4131 (2018)
7. Zhao, S.; Li, Y.; Liu, D.; Liu, J.; Liu, Y.-M.; Zakharov, D. N.; Wu, Q.; Orlov, A.; Gewirth, A. A.; Stach, E. A.; Nuzzo, R. G.; Frenkel, A. I.

- Multimodal study of the speciations and activities of supported Pd catalysts during the hydrogenation of ethylene* J. Phys. Chem. C., **121**, 18962-18972 (2017)
8. Stach, E. A.; Zhao, S.; Li, Y.; Liu, D.; Liu, J.; Liu, Y.-M.; Zakharov, D. N.; Wu, Q.; Orlov, A.; Gewirth, A. A.; Nuzzo, R. G.; Frenkel, A. I. *Operando and multimodal studies of speciation and activity of Pt catalysts during the hydrogenation of ethylene* Microsc. Microanal., **23** (Suppl. 1), 892-893 (2017)
 9. Vila, F. D.; Rehr, J. J.; Nuzzo, R. G.; Frenkel, A. I. *Anomalous structural disorder in supported Pt nanoparticles* J. Phys. Chem. Lett. **8**, 3284-3288 (2017)
 10. Timoshenko, J.; Halder, A.; Yang, B.; Seifert, S.; Pellin, N.; Vajda, S.; Frenkel, A. I. *Subnanometer substructures in nanoassemblies formed from clusters under a reactive atmosphere revealed using machine learning* J. Phys. Chem. C **122**, 21686-21693 (2018)
 11. Timoshenko, J.; Anspoks, A.; Cintins, A.; Kuzmin, A.; Purans, J.; Frenkel, A. I. *Artificial neural network approach for characterizing structural transformations by X-ray absorption fine structure spectroscopy* Phys. Rev. Lett. **120**, 225502 (2018)
 12. Timoshenko, J.; Lu, D.; Lin, Y.; Frenkel, A. I. *Supervised machine learning-based determination of three-dimensional structure of metallic nanoparticles* J. Phys. Chem. Lett., **8**, 5091-5098 (2017). **Also included in Virtual Issue on Machine Learning.**
 13. Li, Y.; Rehr, J. J.; Nuzzo, R. G.; Frenkel, A. I., Clusters. In *X-ray absorption spectroscopy and related techniques: International Tables for Crystallography*; Vol. 1. (in press)
 14. Timoshenko, J.; Roese, S.; Hovel, H.; Frenkel, A. I. *Silver clusters shape determination from in-situ XANES data* Rad. Chem. Phys. **174**, 108049 (2020)
 15. Huang, P.; Huang, J.; Pantovich, S.; Fenton, T.; Carl, A.; Caputo, C.; Grimm, R.; Frenkel, A. I.; Li, G. *Selective CO₂ reduction catalyzed by single cobalt sites on carbon nitride under visible-light irradiation*. J. Am. Chem. Soc. **140**, 16042-16047 (2018)
 16. Zhang, S.; Li, Y.; Huang, J.; Lee, J.; Kim, D. H.; Frenkel, A. I.; Kim, T. *Molecular and electronic structure effects of CoOx/CeO₂ catalysts for the NO reduction by CO*. J. Phys. Chem. C. **123**, 7166-7177 (2019)
 17. Kottwitz, M.; Li, Y.; Huang, J.; Balasubramanian, M.; Lu, D.; Timoshenko, J.; Palomino, R. M.; Senanayake, S. D.; Nuzzo, R. G.; Frenkel, A. I. *Synthesis and characterization of singly dispersed Pt atoms on ceria*. ACS Catalysis **9**, 8738-8748 (2019)
 18. Zhang, W.; Topsakal, M.; Cama, C.; Pelliccione, C.; Zhao, H.; Ehrlich, S.; Wu, L.; Zhu, Y.; Frenkel, A. I.; Takeuchi, K.; Takeuchi, E.; Marschilok, A.; Lu, D.; Wang, F; *Multi-stage structural transformation in zero-strain Lithium Titanate unveiled by in-situ X-ray Absorption fingerprints*. J. Am. Chem. Soc. **2017**. 139 (46), pp 16591–16603 DOI: 10.1021/jacs.7b07628
 19. Zhang, S.; Tang, Y.; Nguyen, L.; Zhao, Y.; Wu, Z.; Goh, T.; Liu, J.; Li, Y.; Zhu, T.; Huang, W.; Frenkel, A. I.; Li, J.; Tao, F., *Catalysis on singly dispersed Rh atoms anchored on an inert support*. ACS Catalysis **2018 (8)**, 110-121. (in press) DOI: 10.1021/acscatal.7b01788
 20. Timoshenko, J.; Lu, D.; Lin, Y.; Frenkel, A. I., *Supervised machine learning-based determination of three-dimensional structure of metallic nanoparticles*. J. Phys. Chem. Lett. **2017**, 8 (20), 5091-5098 DOI: 10.1021/acs.jpcclett.7b02364
 21. Stach, E. A.; Zhao, S.; Li, Y.; Liu, D.; Liu, J.; Liu, Y.-M.; Zakharov, D.; Wu, Q.; Orlov, A.; Gewirth, A.; Nuzzo, R. G.; Frenkel, A. I., *Operando and multimodal studies of speciation and activity of Pt catalysts during the hydrogenation of ethylene*. Microsc. Microanalysis **2017**. 23(1), 892-893 DOI: 10.1017/S1431927617005128
 22. Zhao, S.; Li, Y.; Liu, D.; Liu, J.; Liu, Y.-M.; Zakharov, D.; Wu, Q.; Orlov, A.; Gewirth, A.; Stach, E. A.; Nuzzo, R. G.; Frenkel, A. I., *Multimodal study of the speciations and activities of supported Pd catalysts during the hydrogenation of ethylene*. J. Phys. Chem. C **2017**, 121(34), 18962-18972 DOI: 10.1021/acs.jpcc.7b06270
 23. Wang, Q.; I. Frenkel, A., *Characterization of Model Nanocatalysts by X-ray Absorption Spectroscopy*. 2017; Vol. 177, p 149-183 DOI: 10.1016/B978-0-12-805090-3.00005-X

24. Vila, F. D.; Rehr, J. J.; Nuzzo, R. G.; Frenkel, A. I., Anomalous Structural Disorder in Supported Pt Nanoparticles. *The Journal of Physical Chemistry Letters* **2017**, 8 (14), 3284-3288. DOI: 10.1021/acs.jpcllett.7b01446
25. Shan, J.; Zhang, S.; Choksi, T.; Nguyen, L.; Bonifacio, C. S.; Li, Y.; Zhu, W.; Tang, Y.; Zhang, Y.; Yang, J. C.; Greeley, J.; Frenkel, A. I.; Tao, F., Tuning Catalytic Performance through a Single or Sequential Post-Synthesis Reaction(s) in a Gas Phase. *ACS Catalysis* **2017**, 7 (1), 191-204 DOI: 10.1021/acscatal.6b02054
26. Oezaslan, M.; Herrmann, A.-K.; Werheid, M.; Frenkel, A. I.; Nachtegaal, M.; Dosche, C.; Laugier Bonnaud, C.; Yilmaz, H. C.; Kühn, L.; Rhiel, E.; Gaponik, N.; Eychmüller, A.; Schmidt, T. J., Structural Analysis and Electrochemical Properties of Bimetallic Palladium–Platinum Aerogels Prepared by a Two-Step Gelation Process. *ChemCatChem* **2017**, 9 (5), 798-808 DOI: 10.1002/cctc.201600667
27. Merrill, N. A.; Nitka, T. T.; McKee, E. M.; Merino, K. C.; Drummy, L. F.; Lee, S.; Reinhart, B.; Ren, Y.; Munro, C. J.; Pylypenko, S.; Frenkel, A. I.; Bedford, N. M.; Knecht, M. R., Effects of Metal Composition and Ratio on Peptide-Templated Multimetallic PdPt Nanomaterials. *ACS Applied Materials & Interfaces* **2017**, 9 (9), 8030-8040 DOI: 10.1021/acsami.6b11651
28. Frenkel, A. I.; Li, Y., Metal Nanocatalysts. In *XAFS Techniques for Catalysts, Nanomaterials and Surfaces*, Springer: **2017**; pp 273-298 DOI: 10.1007/978-3-319-43866-5_19
29. Bare, S. R.; Vila, F. D.; Charochak, M. E.; Prabhakar, S.; Bradley, W. J.; Jaye, C.; Fischer, D. A.; Hayashi, S. T.; Bradley, S. A.; Rehr, J. J., Characterization of Coke on a Pt-Re/ γ -Al₂O₃ Reforming Catalyst: Experimental and Theoretical Study. *ACS Catalysis* **2017**, 7 (2), 1452-1461 DOI: 10.1021/acscatal.6b02785
30. Wu, Q.; Ridge, C. J.; Zhao, S.; Zakharov, D.; Cen, J.; Tong, X.; Connors, E.; Su, D.; Stach, E. A.; Lindsay, C. M.; Orlov, A., Development of a New Generation of Stable, Tunable, and Catalytically Active Nanoparticles Produced by the Helium Nanodroplet Deposition Method. *The Journal of Physical Chemistry Letters* **2016**, 7 (15), 2910-2914. DOI: 10.1021/acs.jpcllett.6b01305
31. Vila, F. D.; Hayashi, S. T.; Moore, J. M.; Rehr, J. J., Molecular Dynamics Simulations of Supported Pt Nanoparticles with a Hybrid Sutton–Chen Potential. *The Journal of Physical Chemistry C* **2016**, 120 (27), 14883-14891. DOI: 10.1021/acs.jpcc.6b03074
32. Tao, F. F.; Nguyen, L.; Zhang, S.; Li, Y.; Tang, Y.; Zhang, L.; Frenkel, A. I.; Xia, Y.; Salmeron, M., Formation of Second-Generation Nanoclusters on Metal Nanoparticles Driven by Reactant Gases. *Nano Letters* **2016**, 16 (8), 5001-5009. DOI: 10.1021/acs.nanolett.6b01718
33. Senanayake, S. D.; Pappoe, N. A.; Nguyen-Phan, T.-D.; Luo, S.; Li, Y.; Xu, W.; Liu, Z.; Mudiyansele, K.; Johnston-Peck, A. C.; Frenkel, A. I.; Heckler, I.; Stacchiola, D.; Rodriguez, J. A., Interfacial Cu⁺ promoted surface reactivity: Carbon monoxide oxidation reaction over polycrystalline copper–titania catalysts. *Surface Science* **2016**, 652, 206-212. DOI: 10.1016/j.susc.2016.02.014
34. Oezaslan, M.; Liu, W.; Nachtegaal, M.; Frenkel, A. I.; Rutkowski, B.; Werheid, M.; Herrmann, A. K.; Laugier-Bonnaud, C.; Yilmaz, H. C.; Gaponik, N.; Czyrska-Filemonowicz, A.; Eychmüller, A.; Schmidt, T. J., Homogeneity and elemental distribution in self-assembled bimetallic Pd-Pt aerogels prepared by a spontaneous one-step gelation process. *Physical Chemistry Chemical Physics* **2016**, 18 (30), 20640-20650. DOI: 10.1039/C6CP03527B.
35. Nguyen, L.; Zhang, S.; Wang, L.; Li, Y.; Yoshida, H.; Patlolla, A.; Takeda, S.; Frenkel, A. I.; Tao, F., Reduction of Nitric Oxide with Hydrogen on Catalysts of Singly Dispersed Bimetallic Sites Pt₁Co and Pd₁Co. *ACS Catalysis* **2016**, 6 (2), 840-850. DOI: 10.1021/acscatal.5b00842
36. Lwin, S.; Li, Y.; Frenkel, A. I.; Wachs, I. E., Nature of WO_x Sites on SiO₂ and Their Molecular Structure–Reactivity/Selectivity Relationships for Propylene Metathesis. *ACS Catalysis* **2016**, 6 (5), 3061-3071. DOI: 10.1021/acscatal.6b00389
37. Keturakis, C. J.; Zhu, M.; Gibson, E. K.; Daturi, M.; Tao, F.; Frenkel, A. I.; Wachs, I. E., Dynamics of CrO₃–Fe₂O₃ Catalysts during the High-Temperature Water-Gas Shift Reaction:

Molecular Structures and Reactivity. *ACS Catalysis* **2016**, 6 (7), 4786-4798.

DOI: 10.1021/acscatal.6b01281

38. Huang, W.; Zhang, S.; Tang, Y.; Li, Y.; Nguyen, L.; Li, Y.; Shan, J.; Xiao, D.; Gagne, R.; Frenkel, A. I.; Tao, F., Low-Temperature Transformation of Methane to Methanol on Pd₁O₄ Single Sites Anchored on the Internal Surface of Microporous Silicate. *Angewandte Chemie International Edition* **2016**, 55 (43), 13441-13445. **DOI:** 10.1002/anie.201604708
39. Gänzler, A. M.; Lichtenberg, H.; Frenkel, A. I.; Casapu, M.; Boubnov, A.; Wang, D.; Grunwaldt, J. D., Using combined XAS/DRIFTS to study CO/NO Oxidation over Pt/Al₂O₃ catalysts. *Journal of Physics: Conference Series* **2016**, 712 (1), 012045. **DOI:** 10.1088/1742-6596/712/1/012045
40. Zhu, Q.; Saidi, W. A.; Yang, J. C., Step-Induced Oxygen Upward Diffusion on Stepped Cu(100) Surface. *The Journal of Physical Chemistry C* **2015**, 119 (1), 251-261. **DOI:** 10.1021/jp507914r
41. Zhao, S.; Li, Y.; Stavitski, E.; Tappero, R.; Crowley, S.; Castaldi, M. J.; Zakharov, D. N.; Nuzzo, R. G.; Frenkel, A. I.; Stach, E. A., Operando Characterization of Catalysts through use of a Portable Microreactor. *ChemCatChem* **2015**, 7 (22), 3683-3691. **DOI:** 10.1002/cctc.201500688
42. Zhang, S.; Nguyen, L.; Liang, J.-X.; Shan, J.; Liu, J.; Frenkel, A. I.; Patlolla, A.; Huang, W.; Li, J.; Tao, F., Catalysis on singly dispersed bimetallic sites. *Nature Communications* **2015**, 6, 7938. **DOI:**10.1038/ncomms8938
43. Wang, J.; Wang, Q.; Jiang, X.; Liu, Z.; Yang, W.; Frenkel, A. I., Determination of Nanoparticle Size by Measuring the Metal–Metal Bond Length: The Case of Palladium Hydride. *The Journal of Physical Chemistry C* **2015**, 119 (1), 854-861. **DOI:** 10.1021/jp510730a
44. Stach, E. A.; Li, Y.; Zhao, S.; Gamalski, A.; Zakharov, D.; Tappero, R.; Chen-Weigart, K.; Thieme, J.; Jung, U.; Elsen, A.; Wu, Q.; Orlov, A.; Chen, J.; Nuzzo, R. G.; Frenkel, A., Characterizing Working Catalysts with Correlated Electron and Photon Probes. *Microscopy and Microanalysis* **2015**, 21 (S3), 563-564. **DOI:**10.1017/S143192761500361X
45. Merrill, N. A.; McKee, E. M.; Merino, K. C.; Drummy, L. F.; Lee, S.; Reinhart, B.; Ren, Y.; Frenkel, A. I.; Naik, R. R.; Bedford, N. M.; Knecht, M. R., Identifying the Atomic-Level Effects of Metal Composition on the Structure and Catalytic Activity of Peptide-Templated Materials. *ACS Nano* **2015**, 9 (12), 11968-11979. **DOI:** 10.1021/acsnano.5b04665
46. Lwin, S.; Li, Y.; Frenkel, A. I.; Wachs, I. E., Activation of Surface ReOx Sites on Al₂O₃ Catalysts for Olefin Metathesis. *ACS Catalysis* **2015**, 5 (11), 6807-6814. **DOI:** 10.1021/acscatal.5b01944
47. Lwin, S.; Keturakis, C.; Handzlik, J.; Sautet, P.; Li, Y.; Frenkel, A. I.; Wachs, I. E., Surface ReOx Sites on Al₂O₃ and Their Molecular Structure–Reactivity Relationships for Olefin Metathesis. *ACS Catalysis* **2015**, 5 (3), 1432-1444. **DOI:** 10.1021/cs5016518
48. Liu, H.; An, W.; Li, Y.; Frenkel, A. I.; Sasaki, K.; Koenigsmann, C.; Su, D.; Anderson, R. M.; Crooks, R. M.; Adzic, R. R.; Liu, P.; Wong, S. S., In Situ Probing of the Active Site Geometry of Ultrathin Nanowires for the Oxygen Reduction Reaction. *Journal of the American Chemical Society* **2015**, 137 (39), 12597-12609. **DOI:** 10.1021/jacs.5b07093
49. Li, Y.; Zakharov, D.; Zhao, S.; Tappero, R.; Jung, U.; Elsen, A.; Baumann, P.; Nuzzo, R. G.; Stach, E. A.; Frenkel, A. I., Complex structural dynamics of nanocatalysts revealed in Operando conditions by correlated imaging and spectroscopy probes. *Nature Communications* **2015**, 6, 7583. **DOI:**10.1038/ncomms8583
50. Jung, U.; Elsen, A.; Li, Y.; Smith, J. G.; Small, M. W.; Stach, E. A.; Frenkel, A. I.; Nuzzo, R. G., Comparative in Operando Studies in Heterogeneous Catalysis: Atomic and Electronic Structural Features in the Hydrogenation of Ethylene over Supported Pd and Pt Catalysts. *ACS Catalysis* **2015**, 5 (3), 1539-1551. **DOI:** 10.1021/cs501846g
51. Frenkel, A. I., Two views at strained nanocrystals from the opposite sides of spatial resolution limit. *Physica Scripta* **2015**, 90 (9), 098004. **DOI:** 10.1088/0031-8949/90/9/098004
52. Elsen, A.; Jung, U.; Vila, F.; Li, Y.; Safonova, O. V.; Thomas, R.; Tromp, M.; Rehr, J. J.; Nuzzo, R. G.; Frenkel, A. I., Intracuster Atomic and Electronic Structural Heterogeneities in Supported

Nanoscale Metal Catalysts. *The Journal of Physical Chemistry C* **2015**, *119* (45), 25615-25627. DOI: 10.1021/acs.jpcc.5b08267

53. Crooks, A. B.; Yih, K.-H.; Li, L.; Yang, J. C.; Özkar, S.; Finke, R. G., Unintuitive Inverse Dependence of the Apparent Turnover Frequency on Precatalyst Concentration: A Quantitative Explanation in the Case of Ziegler-Type Nanoparticle Catalysts Made from [(1,5-COD)Ir(μ -O₂C₈H₁₅)₂] and AlEt₃. *ACS Catalysis* **2015**, *5* (6), 3342-3353. DOI: 10.1021/acscatal.5b00347
54. Briggs, B. D.; Bedford, N. M.; Seifert, S.; Koerner, H.; Ramezani-Dakhel, H.; Heinz, H.; Naik, R. R.; Frenkel, A. I.; Knecht, M. R., Atomic-scale identification of Pd leaching in nanoparticle catalyzed C-C coupling: effects of particle surface disorder. *Chemical Science* **2015**, *6* (11), 6413-6419. DOI: 10.1039/C5SC01424G
55. Bonifacio, C. S.; Carenco, S.; Wu, C. H.; House, S. D.; Bluhm, H.; Yang, J. C., Thermal Stability of Core-Shell Nanoparticles: A Combined in Situ Study by XPS and TEM. *Chemistry of Materials* **2015**, *27* (20), 6960-6968. DOI: 10.1021/acs.chemmater.5b01862
56. Bedford, N. M.; Ramezani-Dakhel, H.; Slocik, J. M.; Briggs, B. D.; Ren, Y.; Frenkel, A. I.; Petkov, V.; Heinz, H.; Naik, R. R.; Knecht, M. R., Elucidation of Peptide-Directed Palladium Surface Structure for Biologically Tunable Nanocatalysts. *ACS Nano* **2015**, *9* (5), 5082-5092. DOI: 10.1021/acsnano.5b00168
57. Frenkel, A. I., Applications of extended X-ray absorption fine-structure spectroscopy to studies of bimetallic nanoparticle catalysts. *Chem. Soc. Rev.* **2012**, *41*, 8163-8178.
58. Patlolla, A.; Carino, E. V.; Ehrlich, S. N.; Stavitski, E.; Frenkel, A. I., Application of Operando XAS, XRD, and Raman Spectroscopy for Phase Speciation in Water Gas Shift Reaction Catalysts. *ACS Catal.* **2012**, *2*, 2216-2223.
59. Yang, J. C.; Small, M. W.; Grieshaber, R. V.; Nuzzo, R. G., Recent developments and applications of electron microscopy to heterogeneous catalysis. *Chem. Soc. Rev.* **2012**, *41*, 8179-8194.
60. Small, M. W.; Sanchez, S. I.; Marinkovic, N. S.; Frenkel, A. I.; Nuzzo, R. G., Influence of Adsorbates on the Electronic Structure, Bond Strain, and Thermal Properties of an Alumina-Supported Pt Catalyst. *ACS Nano* **2012**, *6*, 5583-5595.
61. Ryu, H.; Lei, H.; Frenkel, A. I.; Petrovic, C., Local structural disorder and superconductivity in KxFe₂-ySe₂. *Phys. Rev. B.* **2012**, *85*, 224515.
62. Chen, W. F.; Sasaki, K.; Ma, C.; Frenkel, A. I.; Marinkovic, N.; Muckerman, J. T.; Zhu, Y.; Adzic, R. R., Hydrogen-evolution catalysts based on non-noble metal nickel-molybdenum nitride nanosheets. *Angew Chem Int Ed Engl* **2012**, *51*, 6131-5.
63. Zhang, Z.; Jung, K.; Li, L.; Yang, J. C., Kinetics aspects of initial stage thin γ -Al₂O₃ film formation on single crystalline β -NiAl (110). *J. Appl. Phys.* **2012**, *111*, 034312.
64. Zhang, Z.; Gleeson, B.; Jung, K.; Li, L.; Yang, J. C., A diffusion analysis of transient subsurface γ' -Ni₃Al formation during β -NiAl oxidation. *Acta Mater.* **2012**, *60*, 5273-5283.
65. Frenkel, A. I.; Small, M. W.; Smith, J. G.; Nuzzo, R. G.; Kvashnina, K. O.; Tromp, M., An in Situ Study of Bond Strains in 1 nm Pt Catalysts and Their Sensitivities to Cluster-Support and Cluster-Adsorbate Interactions. *J. Phys. Chem. C* **2013**, *117*, 23286-23294.
66. Frenkel, A. I.; Wang, Q.; Sanchez, S. I.; Small, M. W.; Nuzzo, R. G., Short range order in bimetallic nanoalloys: an extended X-ray absorption fine structure study. *J Chem Phys* **2013**, *138*, 064202.
67. Li, L.; Wang, L.-L.; Johnson, D. D.; Zhang, Z.; Sanchez, S. I.; Kang, J. H.; Nuzzo, R. G.; Wang, Q.; Frenkel, A. I.; Li, J.; Ciston, J.; Stach, E. A.; Yang, J. C., Noncrystalline-to-Crystalline Transformations in Pt Nanoparticles. *J. Am. Chem. Soc.* **2013**, *135*, 13062-13072.
68. Merte, L. R.; Ahmadi, M.; Behafarid, F.; Ono, L. K.; Lira, E.; Matos, J.; Li, L.; Yang, J. C.; Roldan Cuenya, B., Correlating Catalytic Methanol Oxidation with the Structure and Oxidation State of Size-Selected Pt Nanoparticles. *ACS Catal.* **2013**, *3*, 1460-1468.
69. Rehr, J. J.; Vila, F. D., Shake-Rattle-and-Roll: A Model of Dynamic Structural Disorder in Supported Nanoscale Catalysts. *ArXiv e-prints* **2013**, *1309*, 1493.

70. Stach, E. A.;Baumann, P.;Li, Y.;Zakharov, D.;Frenkel, A. I., Using operando methods to characterize working catalysts with TEM, XAS, EXAFS and Raman Spectroscopy *Microsc. Microanal.* **2013**, *19*, 1674-1675.
71. Stach, E. A.;Zakharov, D.;Akatay, M. C.;Baumann, P.;Ribeiro, F.;Zvienevich, Y.;Li, Y.;Frenkel, A. I., Developments in environmental transmission electron microscopy for catalysis research. *Microsc. Microanal.* **2013**, *19*, 1174-1175.
72. Zhang, S.;Shan, J.-j.;Zhu, Y.;Frenkel, A. I.;Patlolla, A.;Huang, W.;Yoon, S. J.;Wang, L.;Yoshida, H.;Takeda, S.;Tao, F., WGS Catalysis and In Situ Studies of CoO_{1-x}, PtCon/Co₃O₄, and Pt_mCo_{m'}/CoO_{1-x} Nanorod Catalysts. *J. Am. Chem. Soc.* **2013**, *135*, 8283-8293.
73. Zhang, S.;Tao, F.;Frenkel, A. I.;Takeda, S., Singly anchored Pt and Pd atoms on Co₃O₄ and their catalytic performance *Microsc. Microanal.* **2013**, *19*, 1620-1621
74. Zhang, Z.;Li, L.;Yang, J. C., Adhesion of Pt Nanoparticles Supported on γ -Al₂O₃Single Crystal. *J. Phys. Chem. C* **2013**, *117*, 21407-21412.
75. Erickson, E. M.;Oruc, M. E.;Wetzel, D. J.;Cason, M. W.;Hoang, T. T. H.;Small, M. W.;Li, D.;Frenkel, A. I.;Gewirth, A. A.;Nuzzo, R. G., A Comparison of Atomistic and Continuum Approaches to the Study of Bonding Dynamics in Electrocatalysis: Microcantilever Stress and in Situ EXAFS Observations of Platinum Bond Expansion Due to Oxygen Adsorption during the Oxygen Reduction Reaction. *Anal. Chem.* **2014**, *86*, 8368-8375.
76. Frenkel, A. I.;Cason, M. W.;Elsen, A.;Jung, U.;Small, M. W.;Nuzzo, R. G.;Vila, F. D.;Rehr, J. J.;Stach, E. A.;Yang, J. C., Critical review: Effects of complex interactions on structure and dynamics of supported metal catalysts. *J. Vac. Sci. Technol., A* **2014**, *32*, 020801.
77. Frenkel, A. I.;van Bokhoven, J. A., X-ray spectroscopy for chemical and energy sciences: the case of heterogeneous catalysis. *J. Synchrotron Radiat.* **2014**, *21*, 1084-1089.
78. Patete, J. M.;Han, J.;Tiano, A. L.;Liu, H.;Han, M.-G.;Simonson, J. W.;Li, Y.;Santulli, A. C.;Aronson, M. C.;Frenkel, A. I.;Zhu, Y.;Wong, S. S., Observation of Ferroelectricity and Structure-Dependent Magnetic Behavior in Novel One-Dimensional Motifs of Pure, Crystalline Yttrium Manganese Oxides. *J. Phys. Chem. C* **2014**, *118*, 21695-21705.
79. Rehr, J. J.;Vila, F. D., Dynamic structural disorder in supported nanoscale catalysts. *J. Chem. Phys.* **2014**, *140*, 134701.
80. Shan, J.;Huang, W.;Nguyen, L.;Yu, Y.;Zhang, S.;Li, Y.;Frenkel, A. I.;Tao, F., Conversion of Methane to Methanol with a Bent Mono(μ -oxo)dinickel Anchored on the Internal Surfaces of Micropores. *Langmuir* **2014**, *30*, 8558-8569.
81. Small, M. W.;Kas, J. J.;Kvashnina, K. O.;Rehr, J. J.;Nuzzo, R. G.;Tromp, M.;Frenkel, A. I., Effects of Adsorbate Coverage and Bond-Length Disorder on the d-Band Center of Carbon-Supported Pt Catalysts. *ChemPhysChem* **2014**, *15*, 1569-1572.
82. Zhang, L.;Yang, C.;Frenkel, A. I.;Wang, S.;Xiao, G.;Brinkman, K.;Chen, F., Co-generation of electricity and chemicals from propane fuel in solid oxide fuel cells with anode containing nano-bimetallic catalyst. *J. Power Sources* **2014**, *262*, 421-428.
83. Frenkel, A. I.;Rodriguez, J. A.;Chen, J. G., Synchrotron Techniques for In Situ Catalytic Studies: Capabilities, Challenges, and Opportunities. *ACS Catal.* **2012**, *2*, 2269-2280.
84. Luo, L. L.;Kang, Y. H.;Yang, J. C.;Zhou, G. W., Effect of oxygen gas pressure on orientations of Cu₂O nuclei during the initial oxidation of Cu(100), (110) and (111). *Surf. Sci.* **2012**, *606*, 1790-1797.
85. Vinson, J.;Rehr, J. J., Ab initio Bethe-Salpeter calculations of the x-ray absorption spectra of transition metals at the L-shell edges. *Phys. Rev. B.* **2012**, *86*,
86. Choudhary, V.;Mushrif, S. H.;Ho, C.;Anderko, A.;Nikolakis, V.;Marinkovic, N. S.;Frenkel, A. I.;Sandler, S. I.;Vlachos, D. G., Insights into the Interplay of Lewis and Brønsted Acid Catalysts in Glucose and Fructose Conversion to 5-(Hydroxymethyl)furfural and Levulinic Acid in Aqueous Media. *J. Am. Chem. Soc.* **2013**, *135*, 3997-4006.

87. Corcoran, C. J.;Kang, S.;Li, L.;Guo, X.;Chanda, D.;Nuzzo, R. G., Mechanisms of Enhanced Optical Absorption for Ultrathin Silicon Solar Microcells with an Integrated Nanostructured Backside Reflector. *ACS Appl. Mater. Interfaces* **2013**, 5, 4239-4246.
88. Goldman, J. L.;Cason, M. W.;Wetzel, D. J.;Vieker, H.;Beyer, A.;Gölzhäuser, A.;Gewirth, A. A.;Nuzzo, R. G., Directed Transport as a Route to Improved Performance in Micropore-Modified Encapsulated Multilayer Silicon Electrodes. *J. Electrochem. Soc.* **2013**, 160, A1746-A1752.
89. Long, B. R.;Goldman, J. L.;Nuzzo, R. G.;Gewirth, A. A., Model Ge microstructures as anodes for Li-ion batteries. *J Solid State Electrochem* **2013**, 17, 3015-3020.
90. Yao, Y.;Brueckner, E.;Li, L.;Nuzzo, R., Fabrication and assembly of ultrathin high-efficiency silicon solar microcells integrating electrical passivation and anti-reflection coatings. *Energy Environ. Sci.* **2013**, 6, 3071.
91. Yu, K. J.;Gao, L.;Park, J. S.;Lee, Y. R.;Corcoran, C. J.;Nuzzo, R. G.;Chanda, D.;Rogers, J. A., Light Trapping in Ultrathin Monocrystalline Silicon Solar Cells. *Adv. Energy Mater.* **2013**, 3, 1401-1406.
92. Zhou, G.;Luo, L.;Li, L.;Ciston, J.;Stach, E. A.;Saidi, W. A.;Yang, J. C., In situ atomic-scale visualization of oxide islanding during oxidation of Cu surfaces. *Chem. Comm.* **2013**, 49, 10862-10864.
93. Barile, C. J.;Barile, E. C.;Zavadil, K. R.;Nuzzo, R. G.;Gewirth, A. A., Electrolytic Conditioning of a Magnesium Aluminum Chloride Complex for Reversible Magnesium Deposition. *J. Phys. Chem. C* **2014**, 141107110621009.
94. Braun, P. V.;Nuzzo, R. G., Batteries: Knowing when small is better. *Nature nanotechnology* **2014**,
95. Kas, J. J.;Vila, F. D.;Rehr, J. J.;Chambers, S. A., Real time cumulant approach for charge transfer satellites in x-ray photoemission spectra. *ArXiv e-prints* **2014**, 1408, 2508.
96. Luo, L.;Kang, Y.;Yang, J. C.;Su, D.;Stach, E. A.;Zhou, G., Comparative study of the alloying effect on the initial oxidation of Cu-Au(100) and Cu-Pt(100). *App. Phys. Lett.* **2014**, 104, -.
97. Markiewicz, R. S.;Rehr, J. J.;Bansil, A., Lattice Model of Resonant Inelastic X-Ray Scattering in Metals: Relation of a Strong Core Hole to the X-Ray Edge Singularity. *Phys. Rev. Lett.* **2014**, 112,
98. Story, S. M.;Kas, J. J.;Vila, F. D.;Verstraete, M. J.;Rehr, J. J., Cumulant expansion for phonon contributions to the electron spectral function. *ArXiv e-prints* **2014**, 1407, 6408.
99. Small, M. W.; Sanchez, S. I.; Menard, L. D.; Kang, J. H.; Frenkel, A. I.; Nuzzo, R. G., The Atomic Structural Dynamics of γ -Al₂O₃ Supported Ir-Pt Nanocluster Catalysts Prepared From a Bimetallic Molecular Precursor: A Study Using Aberration-Corrected Electron Microscopy and X-ray Absorption Spectroscopy. *Journal of the American Chemical Society* **2011**,133, 3582-3591.
100. Sasaki, K.; Kuttiyiel, K. A.; Barrio, L.; Su, D.; Frenkel, A. I.; Marinkovic, N.; Mahajan, D.; Adzic, R. R., Carbon-Supported IrNi Core-Shell Nanoparticles: Synthesis, Characterization, and Catalytic Activity. *Journal Of Physical Chemistry C* **2011**,115, 9894-9902.
101. Paredis, K.; Ono, L. K.; Mostafa, S.; Li, L.; Zhang, Z.; Yang, J. C.; Barrio, L.; Frenkel, A. I.; Cuenya, B. R., Structure, chemical composition, and reactivity correlations during the *in-situ* oxidation of 2-propanol. *Journal of the American Chemical Society* **2011**,133, 6728-6735.
102. Paredis, K.; Ono, L. K.; Behafarid, F.; Zhang, Z.; Yang, J. C.; Frenkel, A. I.; Cuenya, B. R., Evolution of the Structure and Chemical State of Pd Nanoparticles during the *in-situ* Catalytic Reduction of NO with H₂. *Journal of the American Chemical Society* **2011**,133, 13455-13464.
103. Marinkovic, N. S.; Wang, Q.; Frenkel, A. I.,*In-situ* diffuse reflectance IR spectroscopy and X-ray absorption spectroscopy for fast catalytic processes. *Journal Of Synchrotron Radiation* **2011**,18, 447-455.
104. Marinkovic, N. S.; Wang, Q.; Barrio, L.; Ehrlich, S. N.; Khalid, S.; Cooper, C.; Frenkel, A. I., Combined *in-situ* X-ray absorption and diffuse reflectance infrared spectroscopy: An attractive tool for catalytic investigations. *Nuclear Instruments & Methods In Physics Research Section A-Accelerators Spectrometers Detectors And Associated Equipment* **2011**,649, 204-206.

105. Li, L.; Zhang, Z.; Ciston, J.; Stach, E. A.; Wang, L.-l.; Johnson, D. D.; Wang, Q.; Frenkel, A. I.; Sanchez, S. I.; Small, M. W.; Nuzzo, R. G.; Yang, J. C., H₂-driven crystallization of supported Pt nanoparticles observed with aberration-corrected Environmental TEM. *Microscopy and Microanalysis* **2011**,17, 1604-1605.
106. Frenkel, A. I.; Yevick, A.; Cooper, C.; Vasic, R., Modeling the Structure and Composition of Nanoparticles by Extended X-Ray Absorption Fine-Structure Spectroscopy. *Annual Review Of Analytical Chemistry, Vol 4* **2011**,4, 23-39.
107. Frenkel, A. I.; Wang, Q.; Marinkovic, N.; Chen, J. G.; Barrio, L.; Si, R.; Lopez Camara, A.; Estrella, A. M.; Rodriguez, J. A.; Hanson, J. C., Combining X-ray Absorption and X-ray Diffraction Techniques for *in-situ* Studies of Chemical Transformations in Heterogeneous Catalysis: Advantages and Limitations. *Journal Of Physical Chemistry C* **2011**,115, 17884-17890.
108. Zhang, Z.; Li, L.; Yang, J. C., γ -Al₂O₃ thin film formation via oxidation of β -NiAl(1 1 0). *Acta Materialia* **2011**,59, 5905-5916.
109. Zhang, Z.; Li, L.; Wang, L.-l.; Sanchez, S. I.; Wang, Q.; Johnson, D. D.; Frenkel, A. I.; Nuzzo, R. G.; Yang, J. C., The Role of γ -Al₂O₃ Single Crystal Support to Pt Nanoparticles Construction. *Microscopy and Microanalysis* **2011**,17, 1324-1325.
110. Erickson, E. M.; Thorum, M. S.; Vasic, R.; Frenkel, A. I.; Gewirth, A. A.; Nuzzo, R. G., In-Situ Electrochemical X-ray Absorbance Spectroscopy Oxygen Reduction Catalysis with High Oxygen Flux. *Journal of the American Chemical Society (Commun.)***2012**, 134, 197-200.
111. Zhang, Z.; Li, L.; Wang, L.-l.; Sanchez, S. I.; Grieshaber, R.; Wang, Q.; Johnson, D. D.; Frenkel, A. I.; Nuzzo, R. G.; Yang, J. C., Preparation and characterization of Pt/ γ -Al₂O₃ model catalyst on NiAl alloy. *Microscopy and Microanalysis* **2010**,16, 1464-1465.
112. Yevick, A.; Frenkel, A. I., Effects of surface disorder on EXAFS modeling of metallic clusters. *Physical Review B* **2010**,81, 115451.
113. Weir, M. G.; Myers, V. S.; Frenkel, A. I.; Crooks, R. M., *In-situ* X-ray Absorption Analysis of similar to 1.8 nm Dendrimer-Encapsulated Pt Nanoparticles during Electrochemical CO Oxidation. *Chemphyschem* **2010**,11, 2942-2950.
114. Sanchez, S. I.; Small, M. W.; Sivaramakrishnan, S.; Wen, J.; Zuo, J.; Nuzzo, R. G., Visualizing Materials Chemistry at Atomic Resolution. *Analytical Chemistry* **2010**,82, 2599-2607.
115. Roldan Cuenya, B.; Croy, J. R.; Mostafa, S.; Behafarid, F.; Li, L.; Zhang, Z.; Yang, J. C.; Wang, Q.; Frenkel, A. I., Solving the Structure of Size-Selected Pt Nanocatalysts Synthesized by Inverse Micelle Encapsulation. *Journal of the American Chemical Society* **2010**,132, 8747-8756.
116. Mostafa, S.; Behafarid, F.; Croy, J. R.; Ono, L. K.; Li, L.; Yang, J. C.; Frenkel, A. I.; Cuenya, B. R., Shape-Dependent Catalytic Properties of Pt Nanoparticles. *Journal of the American Chemical Society* **2010**,132, 15714-15719.
117. Mondloch, J. E.; Wang, Q.; Frenkel, A. I.; Finke, R. G., Development Plus Kinetic and Mechanistic Studies of a Prototype Supported-Nanoparticle Heterogeneous Catalyst Formation System in Contact with Solution: Ir(1,5-COD)Cl/ γ -Al₂O₃ and Its Reduction by H₂ to Ir(0)(n)/ γ -Al₂O₃. *Journal Of The American Chemical Society* **2010**,132, 9701-9714.
118. Li, L.; Zhang, Z.; Croy, J. R.; Mostafa, S.; Cuenya, B. R.; Frenkel, A. I.; Yang, J. C., Ultra-small and Monodisperse Pt nanoparticles supported on γ -Al₂O₃. *Microscopy and Microanalysis* **2010**,16, 1192-1193.
119. Kulkarni, A. D.; Wang, L.; Johnson, D. D.; Sholl, D. S.; Johnson, J. K., First-Principles Characterization of Amorphous Phases of MB12H12, M = Mg, Ca. *Journal Of Physical Chemistry C* **2010**,114, 14601-14605.
120. Khalid, S.; Caliebe, W.; Siddons, P.; So, I.; Clay, B.; Lenhard, T.; Hanson, J.; Wang, Q.; Frenkel, A. I.; Marinkovic, N.; Hould, N.; Ginder-Vogel, M.; Landrot, G. L.; Sparks, D. L.; Ganjoo, A., Quick extended x-ray absorption fine structure instrument with millisecond time scale, optimized for *in-situ* applications. *Review Of Scientific Instruments* **2010**,81, 015105.

121. Finkenstadt, D.; Johnson, D. D., Interphase energies of hcp precipitates in fcc metals: A density-functional theory study in Al-Ag. *Physical Review B* **2010**,*81*, 014113.
122. Alley, W. M.; Hamdemir, I. K.; Wang, Q.; Frenkel, A. I.; Li, L.; Yang, J. C.; Menard, L. D.; Nuzzo, R. G.; Ozkar, S.; Johnson, K. A.; Finke, R. G., Iridium Ziegler-Type Hydrogenation Catalysts Made from [(1,5-COD)Ir(μ -O₂C₈H₁₅)]₂ and AlEt₃: Spectroscopic and Kinetic Evidence for the Irn Species Present and for Nanoparticles as the Fastest Catalyst. *Inorganic Chemistry* **2010**,*49*, 8131-8147.
123. Zheng, J.; Frenkel, A. I.; Wu, L.; Hanson, J.; Ku, W.; Bozin, E. S.; Billinge, S. J. L.; Zhu, Y., Nanoscale disorder and local electronic properties of CaCu₃Ti₄O₁₂: An integrated study of electron, neutron, and x-ray diffraction, x-ray absorption fine structure, and first-principles calculations. *Physical Review B* **2010**,*81*, 144203.
124. Weir, M. G.; Knecht, M. R.; Frenkel, A. I.; Crooks, R. M., Structural Analysis of PdAu Dendrimer-Encapsulated Bimetallic Nanoparticles. *Langmuir* **2010**,*26*, 1137-1146.
125. Dadfarnia, M.; Novak, P.; Ahn, D. C.; Liu, J. B.; Sofronis, P.; Johnson, D. D.; Robertson, I. M., Recent Advances in the Study of Structural Materials Compatibility with Hydrogen. *Advanced Materials* **2010**,*22*, 1128-1135.
126. Zhang, Z.; Li, L.; Wang, L.-l.; Sanchez, S. I.; Grieshaber, R.; Wang, Q.; Johnson, D. D.; Frenkel, A. I.; Nuzzo, R. G.; Yang, J. C., Preparation and characterization of Pt/g-Al₂O₃ model catalyst on NiAl alloy. *Microscopy and Microanalysis* **2010**,*16*, 1464-1465.
127. Yevick, A.; Frenkel, A. I., Effects of surface disorder on EXAFS modeling of metallic clusters. *Physical Review B* **2010**,*81*, 115451.
128. Weir, M. G.; Myers, V. S.; Frenkel, A. I.; Crooks, R. M., *In-situ* X-ray Absorption Analysis of similar to 1.8 nm Dendrimer-Encapsulated Pt Nanoparticles during Electrochemical CO Oxidation. *Chemphyschem* **2010**,*11*, 2942-2950.
129. Sanchez, S. I.; Small, M. W.; Sivaramakrishnan, S.; Wen, J.; Zuo, J.; Nuzzo, R. G., Visualizing Materials Chemistry at Atomic Resolution. *Analytical Chemistry* **2010**,*82*, 2599-2607.
130. Roldan Cuenya, B.; Croy, J. R.; Mostafa, S.; Behafarid, F.; Li, L.; Zhang, Z.; Yang, J. C.; Wang, Q.; Frenkel, A. I., Solving the Structure of Size-Selected Pt Nanocatalysts Synthesized by Inverse Micelle Encapsulation. *Journal of the American Chemical Society* **2010**,*132*, 8747-8756.
131. Mostafa, S.; Behafarid, F.; Croy, J. R.; Ono, L. K.; Li, L.; Yang, J. C.; Frenkel, A. I.; Cuenya, B. R., Shape-Dependent Catalytic Properties of Pt Nanoparticles. *Journal of the American Chemical Society* **2010**,*132*, 15714-15719.
132. Mondloch, J. E.; Wang, Q.; Frenkel, A. I.; Finke, R. G., Development Plus Kinetic and Mechanistic Studies of a Prototype Supported-Nanoparticle Heterogeneous Catalyst Formation System in Contact with Solution: Ir(1,5-COD)Cl/ γ -Al₂O₃ and Its Reduction by H₂ to Ir(0)(n)/ γ -Al₂O₃. *Journal Of The American Chemical Society* **2010**,*132*, 9701-9714.
133. Li, L.; Zhang, Z.; Croy, J. R.; Mostafa, S.; Cuenya, B. R.; Frenkel, A. I.; Yang, J. C., Ultra-small and Monodisperse Pt nanoparticles supported on γ -Al₂O₃. *Microscopy and Microanalysis* **2010**,*16*, 1192-1193.
134. Kulkarni, A. D.; Wang, L.; Johnson, D. D.; Sholl, D. S.; Johnson, J. K., First-Principles Characterization of Amorphous Phases of MB₁₂H₁₂, M = Mg, Ca. *Journal Of Physical Chemistry C* **2010**,*114*, 14601-14605.
135. Khalid, S.; Caliebe, W.; Siddons, P.; So, I.; Clay, B.; Lenhard, T.; Hanson, J.; Wang, Q.; Frenkel, A. I.; Marinkovic, N.; Hould, N.; Ginder-Vogel, M.; Landrot, G. L.; Sparks, D. L.; Ganjoo, A., Quick extended x-ray absorption fine structure instrument with millisecond time scale, optimized for *in-situ* applications. *Review Of Scientific Instruments* **2010**,*81*, 015105.
136. Finkenstadt, D.; Johnson, D. D., Interphase energies of hcp precipitates in fcc metals: A density-functional theory study in Al-Ag. *Physical Review B* **2010**,*81*, 014113.
137. Alley, W. M.; Hamdemir, I. K.; Wang, Q.; Frenkel, A. I.; Li, L.; Yang, J. C.; Menard, L. D.; Nuzzo, R. G.; Ozkar, S.; Johnson, K. A.; Finke, R. G., Iridium Ziegler-Type Hydrogenation

- Catalysts Made from [(1,5-COD)Ir(μ -O₂C₈H₁₅)]₂ and AlEt₃: Spectroscopic and Kinetic Evidence for the Ir^{III} Species Present and for Nanoparticles as the Fastest Catalyst. *Inorganic Chemistry* **2010**,49, 8131-8147.
138. Zheng, J.; Frenkel, A. I.; Wu, L.; Hanson, J.; Ku, W.; Bozin, E. S.; Billinge, S. J. L.; Zhu, Y., Nanoscale disorder and local electronic properties of CaCu₃Ti₄O₁₂: An integrated study of electron, neutron, and x-ray diffraction, x-ray absorption fine structure, and first-principles calculations. *Physical Review B* **2010**,81, 144203.
 139. Weir, M. G.; Knecht, M. R.; Frenkel, A. I.; Crooks, R. M., Structural Analysis of PdAu Dendrimer-Encapsulated Bimetallic Nanoparticles. *Langmuir* **2010**,26, 1137-1146.
 140. Dadfarnia, M.; Novak, P.; Ahn, D. C.; Liu, J. B.; Sofronis, P.; Johnson, D. D.; Robertson, I. M., Recent Advances in the Study of Structural Materials Compatibility with Hydrogen. *Advanced Materials* **2010**,22, 1128-1135.
 141. Zhang, Z.; Li, L.; Wang, L.-l.; Sanchez, S. I.; Wang, Q.; Johnson, D. D.; Frenkel, A. I.; Nuzzo, R. G.; Yang, J. C., Formation and characterization of g-Al₂O₃ films produced by oxidation of b-NiAl[110]. *Microscopy and Microanalysis* **2009**,15, 1440-1441.
 142. Zhang, Z.; Li, L.; Shah, M.; Wen, J.; Yang, J. C., γ -Al₂O₃ Thin Films Catalyst Model Support Preparation on β -NiAl(110) Alloy. *MRS Online Proceedings Library* **2009**,1217, null-null.
 143. Teng, X.; Feygenson, M.; Wang, Q.; He, J.; Du, W.; Frenkel, A. I.; Han, W.; Aronson, M., Electronic and Magnetic Properties of Ultrathin Au/Pt Nanowires. *Nano Letters* **2009**,9, 3177-3184.
 144. Small, M.; Sanchez, S.; Nuzzo, R. G.; Frenkel, A. I., X-ray Absorption Spectroscopy Studies of Model Catalysts. *Synchrotron Radiation News* **2009**,22, 6-11.
 145. Sanchez, S. I.; Small, M. W.; Zuo, J.; Nuzzo, R. G., Structural Characterization of Pt-Pd and Pd-Pt Core-Shell Nanoclusters at Atomic Resolution. *Journal of the American Chemical Society* **2009**,131, 8683-8689.
 146. Sanchez, S. I.; Menard, L. D.; Bram, A.; Kang, J. H.; Small, M. W.; Nuzzo, R. G.; Frenkel, A. I., The Emergence of Nonbulk Properties in Supported Metal Clusters: Negative Thermal Expansion and Atomic Disorder in Pt Nanoclusters Supported on gamma-Al₂O₃. *Journal Of The American Chemical Society* **2009**,131, 7040-7054.
 147. Menard, L. D.; Wang, Q.; Kang, J. H.; Sealey, A. J.; Girolami, G. S.; Teng, X.; Frenkel, A. I.; Nuzzo, R. G., Structural characterization of bimetallic nanomaterials with overlapping x-ray absorption edges. *Physical Review B* **2009**,80, 064111.
 148. Liu, Z.; Hu, J. E.; Wang, Q.; Gaskell, K.; Frenkel, A. I.; Jackson, G. S.; Eichhorn, B., PtMo Alloy and MoOx@Pt Core-Shell Nanoparticles as Highly CO-Tolerant Electrocatalysts. *Journal Of The American Chemical Society* **2009**,131, 6924-+.
 149. Li, L.; Wang, L.-l.; Sanchez, S. I.; Kang, J. H.; Wang, Q.; Zhang, Z.; Frenkel, A. I.; Johnson, D. D.; Nuzzo, R. G.; Yang, J. C., HREM, EXAFS and MD studies on size-dependent crystallinity of Pt nanoparticles supported on g-Al₂O₃. *Microscopy and Microanalysis* **2009**,15, 1210-1211.
 150. Kowal, A.; Li, M.; Shao, M.; Sasaki, K.; Vukmirovic, M. B.; Zhang, J.; Marinkovic, N. S.; Liu, P.; Frenkel, A. I.; Adzic, R. R., Ternary Pt/Rh/SnO₂ electrocatalysts for oxidizing ethanol to CO₂. *Nature Materials* **2009**,8, 325-330.
 151. Karim, A. M.; Prasad, V.; Mpourmpakis, G.; Lonergan, W. W.; Frenkel, A. I.; Chen, J. G.; Vlachos, D. G., Correlating Particle Size and Shape of Supported Ru/gamma-Al₂O₃ Catalysts with NH₃ Decomposition Activity. *Journal Of The American Chemical Society* **2009**,131, 12230-12239.
 152. Grunwaldt, J.-D.; Frenkel, A. I., Synchrotron Studies of Catalysts: From XAFS to QEXAFS and Beyond. *Synchrotron Radiation News* **2009**,22, 2-4.

153. Frenkel, A. I.; Yang, J. C.; Johnson, D. D.; Nuzzo, R. G., Complexity of nanoscale atomic clusters. In *Springer Encyclopedia on Complexity and Systems Science*, Springer: 2009; pp 5589-5912.
154. Finkenstadt, D.; Johnson, D. D., Analysis of nonequilibrium hcp precipitate growth in fcc matrices: Application to Al-Ag. *Materials Science And Engineering A-Structural Materials Properties Microstructure And Processing* **2009**, 525, 174-180.
155. Estrella, M.; Barrio, L.; Zhou, G.; Wang, X.; Wang, Q.; Wen, W.; Hanson, J. C.; Frenkel, A. I.; Rodriguez, J. A., In-situ Characterization of CuFe₂O₄ and Cu/Fe₃O₄ Water-Gas Shift Catalysts. *Journal Of Physical Chemistry C* **2009**, 113, 14411-14417.
156. Wang, L.; Johnson, D. D., Predicted Trends of Core-Shell Preferences for 132 Late Transition-Metal Binary-Alloy Nanoparticles. *Journal Of The American Chemical Society* **2009**, 131, 14023-14029.
157. Wang, L.; Graham, D. D.; Robertson, I. M.; Johnson, D. D., On the Reversibility of Hydrogen-Storage Reactions in Ca(BH₄)₂: Characterization via Experiment and Theory. *Journal Of Physical Chemistry C* **2009**, 113, 20088-20096.
158. Pati, R. K.; Lee, I. C.; Hou, S.; Akhuemonkhan, O.; Gaskell, K. J.; Wang, Q.; Frenkel, A. I.; Chu, D.; Salamanca-Riba, L. G.; Ehrman, S. H., Flame Synthesis of Nanosized Cu-Ce-O, Ni-Ce-O, and Fe-Ce-O Catalysts for the Water-Gas Shift (WGS) Reaction. *Acs Applied Materials & Interfaces* **2009**, 1, 2624-2635.
159. Myers, S. V.; Frenkel, A. I.; Crooks, R. M., X-ray Absorption Study of PdCu Bimetallic Alloy Nanoparticles Containing an Average of similar to 64 Atoms. *Chemistry Of Materials* **2009**, 21, 4824-4829.
160. Liu, J. B.; Johnson, D. D., bcc-to-hcp transformation pathways for iron versus hydrostatic pressure: Coupled shuffle and shear modes. *Physical Review B* **2009**, 79, 134113.
161. Li, H. I.; Pussi, K.; Hanna, K. J.; Wang, L.; Johnson, D. D.; Cheng, H.; Shin, H.; Curtarolo, S.; Moritz, W.; Smerdon, J. A.; McGrath, R.; Diehl, R. D., Surface Geometry of C-60 on Ag(111). *Physical Review Letters* **2009**, 103, 056101.
162. Kibey, S. A.; Wang, L. L.; Liu, J. B.; Johnson, H. T.; Sehitoglu, H.; Johnson, D. D., Quantitative prediction of twinning stress in fcc alloys: Application to Cu-Al. *Physical Review B* **2009**, 79, 214202.
163. Guy, K. A.; Xu, H.; Yang, J. C.; Werth, C. J.; Shapley, J. R., Catalytic nitrate and nitrite reduction with Pd-Cu/PVP colloids in water: Composition, structure, and reactivity correlations. *The Journal of Physical Chemistry C* **2009**, 113, 8177-8185.
164. Bromberg, M. R.; Patlolla, A.; Segal, R.; Feldman, Y.; Wang, Q.; Iqbal, Z.; Frenkel, A. I., Synthesis and characterization of platinum nanoparticles on single-walled Carbon nanotube "nanopaper" support. *Journal of Physics: Conference Series* **2009**, 190, 012155.
165. Alayoglu, S.; Zavalij, P.; Eichhorn, B.; Wang, Q.; Frenkel, A. I.; Chupas, P., Structural and Architectural Evaluation of Bimetallic Nanoparticles: A Case Study of Pt-Ru Core-Shell and Alloy Nanoparticles. *Acs Nano* **2009**, 3, 3127-3137.
166. Alam, A.; Johnson, D. D., Optimal site-centered electronic structure basis set from a displaced-center expansion: Improved results via a priori estimates of saddle points in the density. *Physical Review B* **2009**, 80, 125123.
167. Li, L.; Kang, J. H.; Sanchez, S. I.; Wang, Q.; Wang, L.-l.; Zhang, Z.; Johnson, D. D.; Frenkel, A. I.; Nuzzo, R. G.; Yang, J. C., Size-dependent crystallinity and relative orientations of nano-Pt/ γ -Al₂O₃. *Microscopy and Microanalysis* **2008**, 14, (S02), 184-185.
168. Huang, W. J.; Sun, R.; Tao, J.; Menard, L. D.; Nuzzo, R. G.; Zuo, J. M., Coordination-Dependent Surface Atomic Contraction in Nanocrystals. *Nature Materials*, **2008**, 7, 308 – 313.
169. Petkov, V.; Bedford, N.; Knecht, M. R.; Weir, M. G.; Crooks, R. M.; Tang, W.; Henkelman, G.; Frenkel, A., Periodicity and atomic ordering in nanosized particles of crystals. *Journal of Physical Chemistry C* **2008**, 112, (24), 8907-8911.

170. Teng, X. W.; Han, W. Q.; Wang, Q.; Li, L.; Frenkel, A. I.; Yang, J. C., Hybrid Pt/Au nanowires: Synthesis and electronic structure. *Journal of Physical Chemistry C* **2008**, 112, (38), 14696-14701.
171. Teng, X. W.; Wang, Q.; Liu, P.; Han, W.; Frenkel, A.; Wen, W.; Marinkovic, N.; Hanson, J. C.; Rodriguez, J. A., Formation of Pd/Au nanostructures from Pd nanowires via galvanic replacement reaction. *Journal of the American Chemical Society* **2008**, 130, (3), 1093-1101.
172. Vila, F.; Rehr, J. J.; Kas, J.; Nuzzo, R. G.; Frenkel, A. I., Dynamic structure in supported Pt nanoclusters: Real-time density functional theory and X-ray spectroscopy simulations. *Physical Review B* **2008**, 78, 121404.
173. Wang, L. L.; Johnson, D. D., Electrocatalytic properties of PtBi and PtPb intermetallic line compounds via DFT: CO and H adsorption. *Journal of Physical Chemistry C* **2008**, 112, (22), 8266-8275.
174. Wang, Q.; Hanson, J. C.; Frenkel, A. I., Solving the structure of reaction intermediates by time-resolved synchrotron x-ray absorption spectroscopy. *Journal of Chemical Physics* **2008**, 129, 234502.
175. Dai, B.; Rankin, R. B.; Johnson, J. K.; Allendorf, M. D.; Sholl, D. S.; Zarkevich, N. A.; Johnson, D. D., Influence of Surface Reactions on Complex Hydride Reversibility. *Journal of Physical Chemistry C* **2008**, 112, (46), 18270-18279.
176. Deng, W.; Frenkel, A. I.; Si, R.; Flytzani-Stephanopoulos, M., Reaction-relevant gold structures in the low temperature water-gas shift reaction on Au-CeO₂. *Journal of Physical Chemistry C* **2008**, 112, (33), 12834-12840.
177. Knecht, M. R.; Weir, M. G.; Frenkel, A. I.; Crooks, R. M., Structural rearrangement of bimetallic alloy PdAu nanoparticles within dendrimer templates to yield core/shell configurations. *Chemistry of Materials* **2008**, 20, (3), 1019-1028.
178. Knecht, M. R.; Weir, M. G.; Myers, V. S.; Pyrz, W. D.; Ye, H. C.; Petkov, V.; Buttrey, D. J.; Frenkel, A. I.; Crooks, R. M., Synthesis and Characterization of Pt Dendrimer-Encapsulated Nanoparticles: Effect of the Template on Nanoparticle Formation. *Chemistry of Materials* **2008**, 33, (16), 5218-5228.
179. Liu, Z.; Guy, K. A.; Shapley, J. R.; Werth, C. J.; Wang, Q.; Frenkel, A. I.; Yang, J. C., Microstructural Characterization of Colloid-Derived Bimetallic Pd-Cu Nanocatalysts Supported on γ -Al₂O₃ for Nitrate Reduction. *Microscopy and Microanalysis* **2008**, 14, (S02), 186-187.
180. Poverenov, E.; Efremenko, I.; Frenkel, A. I.; Ben-David, Y.; Shimon, L. J. W.; Leituss, G.; Konstantinovski, L.; Martin, J. M. L.; Milstein, D., Evidence for a terminal Pt(IV)-oxo complex exhibiting diverse reactivity. *Nature* **2008**, 455, (7216), 1093-1096.
181. Zarkevich, N. A.; Johnson, D. D., Predicting enthalpies of molecular substances: Application to LiBH₄. *Physical Review Letters* **2008**, 100, (4), 040602-4.
182. Zarkevich, N. A.; Tan, T. L.; Wang, L. L.; Johnson, D. D., Low-energy antiphase boundaries, degenerate superstructures, and phase stability in frustrated fcc Ising model and Ag-Au alloys. *Physical Review B* **2008**, 77, 144208.
183. Zarkevich, N. A.; Tan, T. L.; Johnson, D. D., First-principles prediction of phase-segregating alloy phase diagrams and a rapid design estimate of their transition temperatures. *Physical Review B* **2007**, 75, 104203.
184. Frenkel, A. I., Solving the 3D structure of metal nanoparticles *Zeitschrift für Kristallographie* **2007**, 222, (Invited article for the special issue "Structure Studies of Nanocrystals."), 605-611.
185. Frenkel, A. I.; Menard, L. D.; Northrup, P.; Rodriguez, J. A.; Zypman, F.; Glasner, D.; Gao, S.-P.; Xu, H.; Yang, J. C.; Nuzzo, R. G., Geometry and Charge State of Mixed-Ligand Au₁₃ Nanoclusters. *AIP Conf. Proc.* **2007**, 882, 749-751.
186. Glasner, D.; Frenkel, A. I., Geometrical characteristics of regular polyhedra: Application to EXAFS studies of nanoclusters. *AIP Conf. Proc.* **2007**, 882, 746-748.

187. Guliamov, O.; Frenkel, A. I.; Menard, L. D.; Nuzzo, R. G.; Kronik, L., Tangential ligand-induced strain in icosahedral Au₁₃. *J. Am. Chem. Soc. (Communications)* **2007**, 129, (10978-10979).
188. Harris, T.; Soussan, L.; Isseroff, R.; Sun, Y.; Rafailovich, M. H.; Frenkel, A. I., EXAFS studies of palladium nanoparticles: Size control and hydrogenation. *AIP Conf. Proc.* **2007**, 882, 752-754.
189. Li, L.; Menard, L. D.; Xu, F.; Kang, J.; Nuzzo, R. G.; Yang, J. C., Quantitative studies on Au nano-catalysts by STEM and HRTEM. *Microscopy and Microanalysis* **2007**, 13, (S02), 566-567.
190. Li, L.; Menard, L. D.; Xu, F.; Nuzzo, R. G.; Yang, J. C., Quantitative STEM and HRTEM Studies on Au Metallic Nano-Catalysts. *Materials Research Society Symposium Proceedings* **2007**, 1026 (Quantitative Electron Microscopy for Materials Science), (1), C09/1-6.
191. Wang, L. L.; Johnson, D. D., Density functional study of structural trends for late-transition-metal 13-atom clusters. *Physical Review B* **2007**, 75, 235405.
192. Kang, J. H.; Menard, L. D.; Nuzzo, R. G.; Frenkel, A. I., Unusual non-bulk properties in nanoscale materials: Thermal metal-metal bond contraction of gamma-alumina-supported Pt catalysts. *Journal of the American Chemical Society* **2006**, 128, (37), 12068-12069.
193. Menard, L. D.; Gao, S.-P.; Xu, H.; Twisten, R. D.; Harper, A. S.; Song, Y.; Wang, G.; Douglas, A. D.; Yang, J. C.; Frenkel, A. I.; Nuzzo, R. G.; Murray, R. W., Sub-Nanometer Au Monolayer-Protected Clusters Exhibiting Molecule-like Electronic Behavior: Quantitative High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy and Electrochemical Characterization of Clusters with Precise Atomic Stoichiometry. *Journal of Physical Chemistry B* **2006**, 110, (26), 12874-12883.
194. Menard, L. D.; Xu, F.; Nuzzo, R. G.; Yang, J. C., Preparation of TiO₂-supported Au nanoparticle catalysts from a Au₁₃ cluster precursor: Ligand removal using ozone exposure versus a rapid thermal treatment. *Journal of Catalysis* **2006**, 243, (1), 64-73.
195. Menard, L. D.; Xu, H.; Gao, S.-P.; Twisten, R. D.; Harper, A. S.; Song, Y.; Wang, G.; Douglas, A. D.; Yang, J. C.; Frenkel, A. I.; Murray, R. W.; Nuzzo, R. G., Metal Core Bonding Motifs of Monodisperse Icosahedral Au₁₃ and Larger Au Monolayer-Protected Clusters As Revealed by X-ray Absorption Spectroscopy and Transmission Electron Microscopy. *Journal of Physical Chemistry B* **2006**, 110, (30), 14564-14573.
196. Xu, F. T.; Menard, L. D.; Xu, H. P.; Gao, S. P.; Wang, L.-L.; Frenkel, A. I.; Nuzzo, R. G.; Johnson, D. D.; Yang, J. C., Quantitative Study of Au Catalytic Nanoparticles by STEM and HRTEM. *Materials Research Society Symposium Proceedings* **2006**, 900, (Quantitative Electron Microscopy for Materials Science), O04-05/1-6.
197. Yang, J.; Xu, F.; Xu, H.; Menard, L.; Wang, L.-L.; Johnson, D. D.; Nuzzo, R.; Frenkel, A. In *Three-dimensional Structures of Supported Metal Nanoparticles*, 16th International Microscopy Congress, IMC-16, Sapporo, Japan, **2006**; p 1572.
198. Finkenstadt, D.; Johnson, D. D., Solute/defect-mediated pathway for rapid nanoprecipitation in solid solutions: gamma surface analysis in fcc Al-Ag. *Physical Review B* **2006**, 73, 024101.
199. Ghosh, S.; Biava, D. A.; Shelton, W. A.; Johnson, D. D., Systematically exact integrated density-of-states Lloyd's formula for disordered alloys with short-range order. *Physical Review B* **2006**, 73, 085106.
200. Sun, Y.; Frenkel, A. I.; Isseroff, R.; Shonbrun, C.; Forman, M.; Shin, K. W.; Koga, T.; White, H.; Zhang, L. H.; Zhu, Y. M.; Rafailovich, M. H.; Sokolov, J. C., Characterization of palladium nanoparticles by using X-ray reflectivity, EXAFS, and electron microscopy. *Langmuir* **2006**, 22, (2), 807-816.
201. Sun, Y.; Frenkel, A. I.; White, H.; Zhang, L. H.; Zhu, Y. M.; Xu, H. P.; Yang, J. C.; Koga, T.; Zaitsev, V.; Rafailovich, M. H.; Sokolov, J. C., Comparison of decanethiolate gold

- nanoparticles synthesized by one-phase and two-phase methods. *Journal of Physical Chemistry B* **2006**, 110, (46), 23022-23030.
202. Zarkevich, N. A.; Johnson, D. D., Comment on "Structural stability of complex hydrides: LiBH₄ revisited". *Physical Review Letters* **2006**, 97, 119601.
 203. L.-L. Wang, S. V. Khare, D. D. Johnson, A. A. Rockett, V. Chirita, A. I. Frenkel, N. H. Mack, and R. G. Nuzzo "Origin of bulk-like structure and bond distributions of Pt₃₇ and Pt₆Ru₃₁ cluster on carbon: comparison of theory and experiment" *J. Am. Chem. Soc.*, **2006**, 128, 131-142.
 204. Y. Sun, A. I. Frenkel, R. Isseroff, C. Shonbrun, M. Forman, K. Shin, T. Koga, H. White, L. Zhang, Y. Zhu, M. H. Rafailovich, J. C. Sokolov "Characterization of palladium nanoparticles using X-ray reflectivity, EXAFS and electron microscopy" *Langmuir* **2006**, 22, 807-816.
 205. A. I. Frenkel, S. Nemzer, I. Pister, L. Soussan, T. Harris, Y. Sun, M. H. Rafailovich "Size-controlled synthesis and characterization of thiol-stabilized gold nanoparticles" *J. Chem. Phys.* **2005**, 123, 184701.
 206. W. Li, A. I. Frenkel, J. C. Woicik, C. Ni, S. Ismat Shah "Dopant location identification in Nd³⁺-doped TiO₂ nanoparticles" *Phys. Rev. B* **2005**, 72, 155315.
 207. Wang, L.-L.; Johnson, D.D. "Removing critical errors for DFT application to transition-metal nanoclusters: correct ground-state structures of Ru clusters," *J. Phys. Chem. B.* **2005**, 109, 23113-17.
 208. Zarkevich N.; Johnson D.D. "Energy Scaling and Surface Patterning of Halogen-Terminated Si(001) Surfaces," *Surf. Sci. Lett.* **2005**, 591, L292-8.
 209. Wang, G.; Huang, T.; Murray, R. W.; Menard, L.; Nuzzo, R. G. "Near-IR Luminescence of Monolayer-Protected Metal Clusters," *J. Amer. Chem. Soc.* **2005**, 127, 812-813.
 210. H. Xu, R. Twesten, K. Guy, J. Shapley, C. Werth, A. I. Frenkel, D. Johnson, J. Yang "Structural changes of bimetallic Pd(x)Cu(1-x) nanocatalysts developed for nitrate reduction of drinking water", in *Nanoporous and Nanostructured Materials for Catalysis, Sensor and Gas Separation Applications*, Ed. by S. W. Lu, H. Hahn, J. Weismuller, and J. L. Gole Mater. Res. Soc. Symp. Proc. 876E, Warrendale, PA, **2005**, p. R. 4.8.1
 211. H. Xu, L. Menard, A. I. Frenkel, R. Nuzzo, D. Johnson, J. Yang "The effect of substrates/ligands on metal nanocatalysts investigated by quantitative Z Contrast imaging and High Resolution Electron Microscopy" in *Nanoporous and Nanostructured Materials for Catalysis, Sensor and Gas Separation Applications*, ed. by S. W. Lu, H. Hahn, J. Weismuller, and J. L. Gole, *Mater. Res. Soc. Symp. Proc.* 876E, Warrendale, PA, **2005**, p. R9.4/P6.4.
 212. Xu, H.; Menard, L.; Frenkel, A.; Nuzzo, R.; Johnson, D. D.; Yang, J. C., "3-Dimensional Structural Characterization Approaches of Carbon-Supported Au₁₃ Nano-Clusters", *Microscopy & Microanalysis*, **2004**, 10 (suppl 2), 454-456.
 213. X. Wang, J. C. Hanson, A. I. Frenkel, J.-J. Kim, J. A. Rodriguez, "Time-resolved studies of the mechanism of reduction of copper oxides with carbon monoxide: complex behavior of lattice oxygen and the formation of suboxides", *J. Phys. Chem. B* **2004**, 108, 13667.
 214. D. E. Schwarz, A. I. Frenkel, A. Vairavamurthy, R. G. Nuzzo, T. B. Rauchfuss, "Electrosynthesis of ReS₄. XAS analysis of ReS₂, Re₂S₇, and ReS₄" *Chem, Mater.* **2004**, 16, 151-158.

Papers jointly funded by the DOE award and other grants with relatively minor intellectual contribution from the DOE grant:

215. Roese, S.; Kononov, A.; Timoshenko, J.; Frenkel, A. I.; Hovel, H, *Cluster assemblies produced by aggregation of preformed Ag clusters in ionic liquids* *Langmuir* **34**, 4811-4819 (2018)
216. Yan, B.; Wu, Q.; Cen, J.; Timoshenko, J.; Frenkel, A. I.; Su, D.; Chen, X.; Parise, J. B.; Stach, E. A.; Orlov, A.; Chen, J. G. *Highly active subnanometer Rh clusters derived from Rh-doped SrTiO₃ for CO₂ reduction* *Applied Catalysis B: Environmental* **237**, 1003-1011 (2018)

217. Vovchok, D.; Guild, C. J.; Dissanayake, S.; Llorca, J.; Stavitski, E.; Liu, Z.; Palomino, R.; Waluyo, I.; Li, Y.; Frenkel, A. I.; Rodriguez, J. A.; Suib, S. L.; Senanayake, S. D. *Operando characterization of mesoporous Co/CeO₂ catalysts for the high temperature water-gas shift* J. Phys. Chem. C **122**, 8998-9008 (2018)
218. Zhang, F.; Liu, Z.; Zhang, S.; Akter, N.; Palomino, R. M.; Vovchok, D.; Orozco, I.; Salazar, D.; Rodriguez, J. A.; Llorca, J.; Lee, J.; Kim, D. H.; Xu, W.; Frenkel, A. I.; Li, Y.; Kim, T.; Senanayake, S. D. *In situ elucidation of the active state of Co-CeO_x catalysts in the dry reforming of methane: The important role of the reducible oxide support and interactions with Cobalt* ACS Catalysis **8**, 3550-3560 (2018)
219. Tang, Y.; Li, Y.; Fung, V.; Jiang, D.; Huang, W.; Zhang, S.; Iwasawa, Y.; Sakata, T.; Nguyen, L.; Zhang, X.; Frenkel, A. I.; Tao, F. *Single rhodium atoms anchored in micropores for efficient transformation of methane under mild condition* Nature Communications **9**, 1231 (2018)
220. Wu, Q.; Yan, B.; Cen, J.; Timoshenko, J.; Zakharov, D.; Chen, X.; Xin, H.; Yao, S.; Parise, J.; Frenkel, A. I.; Stach, E. A.; Chen, J. G.; Orlov, A. *Growth of Nanocatalyst with Desired Catalytic Functions by Controlled Doping-Segregation of Metal in Oxide* Chem. Mater. **30**, 1585-1592 (2018)
221. Wu, Q.; Cen, J.; Zhao, Y.; Tong, X.; Li, Y.; Frenkel, A. I.; Zhao, S.; Orlov, A. *A comprehensive study of catalytic, morphological and electronic properties of ligand-protected gold nanoclusters using XPS, STM, XAFS and TPD techniques* Phys. Chem. Chem. Phys. **20**, 1497-1503 (2018)
222. Zhang, S.; Tang, Y.; Nguyen, L.; Zhao, Y.-F.; Wu, Z.; Goh, T. W.; Liu, J.; Li, Y.; Zhu, T.; Huang, W.; Frenkel, A. I.; Li, J.; Tao, F. *Catalysis on singly dispersed Rh atoms anchored on an inert support* ACS Catalysis **8**, 110-121 (2018)
223. Rosentsveig, R.; Yadgarov, L.; Feldman, Y.; Shilstein, S.; Popovitz-Biro, R.; Visic, B.; Sedova, A.; Cohen, S. R.; Li, Y.; Frenkel, A. I.; Tenne, R. *Doping of fullerene-like MoS₂ nanoparticles with minute amounts of niobium* Part. Part. Syst. Charact. **35**, 1700165 (2018).
March 25, 2018 Inside Front Cover
224. Zhang, W.; Topsakal, M.; Cama, C.; Pelliccione, C. J.; Zhao, H.; Ehrlich, S.; Wu, L.; Zhu, Y.; Frenkel, A. I.; Takeuchi, K. J.; Takeuchi, E. S.; Marschilok, A. C.; Lu, D.; Wang, F. *Multi-stage structural transformations in zero-strain Lithium Titanate unveiled by in situ X-ray Absorption fingerprints* J. Am. Chem. Soc., **139**, 16591-16603 (2017)
225. Boubnov, A.; Timoshenko, J.; Wrasman, C.; Hoffman, A.; Cargnello, M.; Frenkel, A. I.; Bare, S. R. *Advanced modeling of EXAFS data from Pd-Au nanoparticle catalyst libraries: Comparison of data from SSRL and the APS* Rad. Chem. Phys. **175**, 108304 (2020)
226. Chen-Wiegart, Y.-C. K.; Campbell, S.; Yager, K. G.; Liu, Y.; Frenkel, A. I.; Yang, L.; Bai, J.; McCormick, M.; Allan, D.; Basham, M. *Multi-modal characterization: Overview of modern techniques and data analysis methods* Chapter in “Experimental Analysis Solutions for Leading Experimental Techniques”, World Scientific Series on Emerging Technologies, v.2, Chapter 3, pp. 39-64 (2020).
227. Lin, Y.; Topsakal, M.; Timoshenko, J.; Lu, D.; Yoo, S.; Frenkel, A. I. *Machine-Learning assisted determination of coordination numbers of metallic nanoparticles – A benchmark* Chapter in “Experimental Analysis Solutions for Leading Experimental Techniques”, World Scientific Series on Emerging Technologies, v.2, Chapter 7, pp. 127-140 (2020).
228. Zhao, M.; Xu, Y.; Shuller-Nickles, L.; Amoroso, J.; Frenkel, A. I.; Li, Y.; Gong, W.; Lilova, K.; Navrotsky, A.; Brinkman, K. *Compositional control of radionuclide retention in hollandite-based ceramic waste forms for Cs-immobilization: The role of local structure & thermodynamic stability on elemental release*. J. Am. Cer. Soc. **102**, 4314-4324 (2019)
229. Halder, A.; Lenardi, C.; Yang, B.; Timoshenko, J.; Kolipaka, L.; Seifert, S.; Frenkel, A. I.; Milani, P.; Vajda, S. *CO₂ methanation on Cu cluster decorated zirconia supports with different morphology: a combined in situ XANES and XPS study*. ACS Catalysis **11**, 6210-6224 (2021)

230. Taifan, W. E.; Li, Y.; Baltrus, J. P.; Zhang, L.; Frenkel, A. I.; Baltrusaitis, J. *Operando structure determination of Cu and Zn on supported MgO/SiO₂ catalysts during ethanol conversion to 1,3-butadiene*. *ACS Catalysis* **9**, 269-285 (2019)
231. Korobko, R.; Lerner, A.; Li, Y.; Wachtel, E.; Frenkel, A. I.; Lubomirsky, I., In-situ extended X-ray absorption fine structure study of electrostriction in Gd doped ceria. *Applied Physics Letters* **2015**, *106* (4), 042904. DOI: [10.1063/1.4906857](https://doi.org/10.1063/1.4906857)
232. Li, Y.; Kraynis, O.; Kas, J.; Weng, T.-C.; Sokaras, D.; Zacharowicz, R.; Lubomirsky, I.; Frenkel, A. I., Geometry of electromechanically active structures in Gadolinium - doped Cerium oxides. *AIP Advances* **2016**, *6* (5), 055320. DOI: [10.1063/1.4952645](https://doi.org/10.1063/1.4952645)
233. Korobko, R.; Patlolla, A.; Kossoy, A.; Wachtel, E.; Tuller, H. L.; Frenkel, A. I.; Lubomirsky, I., Giant Electrostriction in Gd-Doped Ceria. *Adv. Mater.* **2012**, *24*, 5857-5861.
234. Lei, H.; Ryu, H.; Ivanovski, V.; Warren, J. B.; Frenkel, A. I.; Cekic, B.; Yin, W.-G.; Petrovic, C., Structure and physical properties of the layered iron oxychalcogenide BaFe₂Se₂O. *Phys. Rev. B* **2012**, *86*, 195133.
235. Lyahovitskaya, V.; Feldman, Y.; Zon, I.; Yoffe, A.; Frenkel, A. I., Strain-arranged structure in amorphous films. *J. Mater. Res.* **2012**, *27*, 2819-2828.
236. Coppage, R.; Slocik, J. M.; Briggs, B. D.; Frenkel, A. I.; Naik, R. R.; Knecht, M. R., Determining Peptide Sequence Effects That Control the Size, Structure, and Function of Nanoparticles. *ACS Nano* **2012**, *6*, 1625-1636.
237. Landon, J.; Demeter, E.; İnoğlu, N.; Keturakis, C.; Wachs, I. E.; Vasić, R.; Frenkel, A. I.; Kitchin, J. R., Spectroscopic Characterization of Mixed Fe-Ni Oxide Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Electrolytes. *ACS Catal.* **2012**, *2*, 1793-1801.
238. Myers, V. S.; Frenkel, A. I.; Crooks, R. M., In Situ Structural Characterization of Platinum Dendrimer-Encapsulated Oxygen Reduction Electrocatalysts. *Langmuir* **2012**, *28*, 1596-1603.
239. Yan, W.; Vasic, R.; Frenkel, A. I.; Koel, B. E., Intraparticle Reduction of Arsenite (As(III)) by Nanoscale Zerovalent Iron (nZVI) Investigated with In Situ X-ray Absorption Spectroscopy. *Environ. Sci. Technol.* **2012**, *46*, 7018-7026.
240. Frenkel, A. I.; Vasić, R.; Dukes, B.; Li, D.; Chen, M.; Zhang, L.; Fujita, T., Thermal properties of nanoporous gold. *Phys. Rev. B* **2012**, *85*,
241. Yadgarov, L.; Rosentsveig, R.; Leituss, G.; Albu-Yaron, A.; Moshkovich, A.; Perfilyev, V.; Vasic, R.; Frenkel, A. I.; Enyashin, A. N.; Seifert, G.; Rapoport, L.; Tenne, R., Controlled doping of MS₂ (M=W, Mo) nanotubes and fullerene-like nanoparticles. *Angew Chem Int Ed Engl* **2012**, *51*, 1148-51.
242. Yih, K. H.; Hamdemir, I. K.; Mondloch, J. E.; Bayram, E.; Ozkar, S.; Vasic, R.; Frenkel, A. I.; Anderson, O. P.; Finke, R. G., Synthesis and characterization of [Ir(1,5-cyclooctadiene)(μ-H)]₄: a tetrametallic Ir₄H₄-core, coordinatively unsaturated cluster. *Inorganic chemistry* **2012**, *51*, 3186-93.
243. Patlolla, A.; Zunino, J.; Frenkel, A. I.; Iqbal, Z., Thermochromism in polydiacetylene-metal oxide nanocomposites. *J. Mater. Chem.* **2012**, *22*, 7028.
244. Amakawa, K.; Sun, L.; Guo, C.; Hävecker, M.; Kube, P.; Wachs, I. E.; Lwin, S.; Frenkel, A. I.; Patlolla, A.; Hermann, K.; Schlögl, R.; Trunschke, A., How Strain Affects the Reactivity of Surface Metal Oxide Catalysts. *Angew Chem Int Ed* **2013**, *52*, 13553-13557.
245. Amit, Y.; Eshet, H.; Faust, A.; Patlolla, A.; Rabani, E.; Banin, U.; Frenkel, A. I., Unraveling the Impurity Location and Binding in Heavily Doped Semiconductor Nanocrystals: The Case of Cu in InAs Nanocrystals. *J. Phys. Chem. C* **2013**, *117*, 13688-13696.
246. Amit, Y.; Faust, A.; Millo, O.; Rabani, E.; Frenkel, A. I.; Banin, U., How to Dope a Semiconductor Nanocrystal *ECS Trans.* **2013**, *58*, 127-133.
247. Anderson, R. M.; Zhang, L.; Loussaert, J. A.; Frenkel, A. I.; Henkelman, G.; Crooks, R. M., An Experimental and Theoretical Investigation of the Inversion of Pd@Pt Core@Shell Dendrimer-Encapsulated Nanoparticles. *ACS Nano* **2013**, *7*, 9345-9353.

248. Frenkel, A. I.;Hanson, J. C., Combined XAFS-XRD methods in Catalysis Research. *In situ Characterization of Heterogeneous Catalysts* **2013**,
249. Frenkel, A. I.;Khalid, S.;Hanson, J. C.;Nachtegaal, M., QEXAFS in Catalysis Research: Principles, Data Analysis and Applications. *In situ Characterization of Heterogeneous Catalysts* **2013**,
250. Kossoy, A.;Wang, Q.;Korobko, R.;Grover, V.;Feldman, Y.;Wachtel, E.;Tyagi, A. K.;Frenkel, A. I.;Lubomirsky, I., Evolution of the local structure at the phase transition in CeO₂-Gd₂O₃ solid solutions. *Phys. Rev. B* **2013**, *87*, 054101.
251. Patlolla, A.;Baumann, P.;Xu, W.;Senanayake, S. D.;Rodriguez, J. A.;Frenkel, A. I., Characterization of Metal-Oxide Catalysts in Operando Conditions by Combining X-ray Absorption and Raman Spectroscopies in the Same Experiment. *Top. Catal.* **2013**, *56*, 896-904.
252. Perelshtein, I.;Ruderman, E.;Perkas, N.;Tzanov, T.;Beddow, J.;Joyce, E.;Mason, T. J.;Blanes, M.;Molla, K.;Patlolla, A.;Frenkel, A. I.;Gedanken, A., Chitosan and chitosan-ZnO-based complex nanoparticles: formation, characterization, and antibacterial activity. *J. Mater. Chem. B* **2013**, *1*, 1968-1976.
253. Sanchez, S. I.;Small, M. W.;Bozin, E. S.;Wen, J. G.;Zuo, J. M.;Nuzzo, R. G., Metastability and structural polymorphism in noble metals: the role of composition and metal atom coordination in mono- and bimetallic nanoclusters. *ACS Nano* **2013**, *7*, 1542-57.
254. Wang, L.;Zhang, S.;Zhu, Y.;Patlolla, A.;Shan, J.;Yoshida, H.;Takeda, S.;Frenkel, A. I.;Tao, F., Catalysis and In Situ Studies of Rh₁/Co₃O₄ Nanorods in Reduction of NO with H₂. *ACS Catal.* **2013**, *3*, 1011-1019.
255. Yancey, D. F.;Chill, S. T.;Zhang, L.;Frenkel, A. I.;Henkelman, G.;Crooks, R. M., A theoretical and experimental examination of systematic ligand-induced disorder in Au dendrimer-encapsulated nanoparticles. *Chem. Sci.* **2013**, *4*, 2912-2921.
256. He, L.;Liu, F.;Hautier, G.;Oliveira, M. J. T.;Marques, M. A. L.;Vila, F. D.;Rehr, J. J.;Rignanese, G.-M.;Zhou, A., Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. *Phys. Rev. B* **2014**, *89*, 64305.
257. Spanjers, C. S.;Senftle, T. P.;van Duin, A. C. T.;Janik, M. J.;Frenkel, A. I.;Rioux, R. M., Illuminating surface atoms in nanoclusters by differential X-ray absorption spectroscopy. *Phys. Chem. Chem. Phys.* **2014**, *16*, 26528-26538
258. Wu, L.-b.;Wu, L.-h.;Yang, W.-m.;Frenkel, A. I., Study of the local structure and oxidation state of iron in complex oxide catalysts for propylene ammoxidation. *Catal. Sci. Technol.* **2014**, *4*, 2512-2519.
259. Carlson, A.;Bowen, A. M.;Huang, Y.;Nuzzo, R. G.;Rogers, J. A., Transfer printing techniques for materials assembly and micro/nanodevice fabrication. *Adv Mater* **2012**, *24*, 5284-318.
260. Guzzo, M.;Kas, J. J.;Sottile, F.;Silly, M. G.;Sirotti, F.;Rehr, J. J.;Reining, L., Plasmon satellites in valence-band photoemission spectroscopy. *Eur. Phys. J. B* **2012**, *85*,
261. Jorissen, K.;Vila, F. D.;Rehr, J. J., A high performance scientific cloud computing environment for materials simulations. *Computer Physics Communications* **2012**, *183*, 1911-1919.
262. Yang, J. C.;Zhou, G., In situ ultra-high vacuum transmission electron microscopy studies of the transient oxidation stage of Cu and Cu alloy thin films. *Micron* **2012**, *43*, 1195-1210.
263. Zhou, G.;Luo, L.;Li, L.;Ciston, J.;Stach, E. A.;Yang, J. C., Step-Edge-Induced Oxide Growth During the Oxidation of Cu Surfaces. *Phys. Rev. Lett.* **2012**, *109*, 235502.
264. Bronstein, N. D.;Li, L.;Xu, L.;Yao, Y.;Ferry, V. E.;Alivisatos, A. P.;Nuzzo, R. G., Luminescent Solar Concentration with Semiconductor Nanorods and Transfer-Printed Micro-Silicon Solar Cells. *ACS Nano* **2013**, *8*, 44-53.
265. Carroll, T. X.;Zahl, M. G.;Borve, K. J.;Saethre, L. J.;Decleva, P.;Ponzi, A.;Kas, J. J.;Vila, F. D.;Rehr, J. J.;Thomas, T. D., Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne. *J Chem Phys* **2013**, *138*, 234310.

266. Feng, X.;Cheng, H.;Bowen, A. M.;Carlson, A. W.;Nuzzo, R. G.;Rogers, J. A., A Finite-Deformation Mechanics Theory for Kinetically Controlled Transfer Printing. *J. Appl. Mech.* **2013**, *80*, 061023-061023.
267. Fister, T. T.;Goldman, J. L.;Long, B. R.;Nuzzo, R. G.;Gewirth, A. A.;Fenter, P. A., X-ray diffraction microscopy of lithiated silicon microstructures. *App. Phys. Lett.* **2013**, *102*, -.
268. Kang, Y.;Luo, L.;Tong, X.;Starr, D.;Zhou, G.;Yang, J., Transient Oxidation of Cu-5at.%Ni(001): Temperature Dependent Sequential Oxide Formation. *Oxid Met* **2013**, *79*, 303-311.
269. Le, A.-P.;Kang, S.;Thompson, L. B.;Rubakhin, S. S.;Sweedler, J. V.;Rogers, J. A.;Nuzzo, R. G., Quantitative Reflection Imaging of Fixed Aplysia californica Pedal Ganglion Neurons on Nanostructured Plasmonic Crystals. *J. Phys. Chem. B* **2013**, *117*, 13069-13081.
270. Sheng, X.;Corcoran, C. J.;He, J.;Shen, L.;Kim, S.;Park, J.;Nuzzo, R. G.;Rogers, J. A., Enhanced ultraviolet responses in thin-film InGaP solar cells by down-shifting. *Phys. Chem. Chem. Phys.* **2013**, *15*, 20434-20437.
271. Sheng, X.;Shen, L.;Kim, T.;Li, L.;Wang, X.;Dowdy, R.;Froeter, P.;Shigeta, K.;Li, X.;Nuzzo, R. G.;Giebink, N. C.;Rogers, J. A., Doubling the Power Output of Bifacial Thin-Film GaAs Solar Cells by Embedding Them in Luminescent Waveguides. *Adv. Energy Mater.* **2013**, *3*, 991-996.
272. Yu, C.;Duan, Z.;Yuan, P.;Li, Y.;Su, Y.;Zhang, X.;Pan, Y.;Dai, L. L.;Nuzzo, R. G.;Huang, Y.;Jiang, H.;Rogers, J. A., Electronically programmable, reversible shape change in two- and three-dimensional hydrogel structures. *Adv Mater* **2013**, *25*, 1541-6.
273. Yuan, P.;Kuksenok, O.;Gross, D. E.;Balazs, A. C.;Moore, J. S.;Nuzzo, R. G., UV patternable thin film chemistry for shape and functionally versatile self-oscillating gels. *Soft Matter* **2013**, *9*, 1231-1243.
274. Ahmed, T.;Haraldsen, J. T.;Rehr, J. J.;Di Ventra, M.;Schuller, I.;Balatsky, A. V., Correlation dynamics and enhanced signals for the identification of serial biomolecules and DNA bases. *Nanotechnol.* **2014**, *25*, 5705.
275. Du, W.;Yang, G.;Wong, E.;Deskins, N. A.;Frenkel, A. I.;Su, D.;Teng, X., Platinum-Tin Oxide Core-Shell Catalysts for Efficient Electro-Oxidation of Ethanol. *J. Am. Chem. Soc.* **2014**, *136*, 10862-10865.
276. Guzzo, M.;Kas, J. J.;Sponza, L.;Giorgetti, C.;Sottile, F.;Pierucci, D.;Silly, M. G.;Sirotti, F.;Rehr, J. J.;Reining, L., Multiple satellites in materials with complex plasmon spectra: From graphite to graphene. *Phys. Rev. B.* **2014**, *89*,
277. Kas, J. J.;Rehr, J. J.;Reining, L., Cumulant expansion of the retarded one-electron Green function. *Phys. Rev. B.* **2014**, *90*,
278. Klevak, E.;Kas, J. J.;Rehr, J. J., Charge transfer satellites in x-ray spectra of transition metal oxides. *Phys. Rev. B.* **2014**, *89*, 85123.
279. Li, L.;Luo, L.;Ciston, J.;Saidi, W. A.;Stach, E. A.;Yang, J. C.;Zhou, G., Surface-Step-Induced Oscillatory Oxide Growth. *Phys. Rev. Lett.* **2014**, *113*, 136104.
280. Schattschneider, P.;Rehr, J. J.;Allen, L. J., Comment on “Electromagnetic Vortex Fields, Spin, and Spin-Orbit Interactions in Electron Vortices”. *Phys. Rev. Lett.* **2014**, *113*,
281. Sheng, X.;Bower, C. A.;Bonafede, S.;Wilson, J. W.;Fisher, B.;Meitl, M.;Yuen, H.;Wang, S.;Shen, L.;Banks, A. R.;Corcoran, C. J.;Nuzzo, R. G.;Burroughs, S.;Rogers, J. A., Printing-based assembly of quadruple-junction four-terminal microscale solar cells and their use in high-efficiency modules. *Nat Mater* **2014**, *13*, 593-598.
282. Zhida, X.;Yuan, Y.;Eric, P. B.;Lanfeng, L.;Jing, J.;Ralph, G. N.;Gang Logan, L., Black silicon solar thin-film microcells integrating top nanocone structures for broadband and omnidirectional light-trapping. *Nanotechnol.* **2014**, *25*, 305301.
283. Shen, X.-F.;Morey, A.;Liu, J.;Ding, Y.-S.;Durand, J.;Wang, Q.;Wen, W.;Hines, W. A.;Hanson, J. C.;Bai, J.;Frenkel, A. I.;Reiff, W.;Aindow, M.;Suib, S. L.;Cai, J.,

Characterization of the Fe-doped mixed-valent tunnel structure manganese oxide KOMS-2
Journal Of Physical Chemistry C **2011**.

284. Piovano, A.; Agostini, G.; Frenkel, A. I.; Bertier, T.; Prestipino, C.; Ceretti, M.; Paulus, W.; Lamberti, C., Time Resolved *in-situ* XAFS Study of the Electrochemical Oxygen Intercalation in SrFeO_{2.5} Brownmillerite Structure: Comparison with the Homologous SrCoO_{2.5} System. *Journal Of Physical Chemistry C* **2011**,115, 1311-1322.
285. Coppage, R.; Slocik, J. M.; Briggs, B. D.; Frenkel, A. I.; Heinz, H.; Naik, R. R.; Knecht, M. R., Crystallographic Recognition Controls Peptide Binding for Bio-Based Nanomaterials. *Journal Of The American Chemical Society* **2011**,133, 12346-12349.
286. H. Lei, H. Ryu, A. I. Frenkel, C. Petrovic Anisotropy in BaFe₂Se₃ single crystals with double chains of FeSe tetrahedra. *Phys. Rev. B*. **2011**, 84, 214511.
287. Du, W.; Wang, Q.; Saxner, D.; Deskins, N. A.; Su, D.; Krzanowski, J. E.; Frenkel, A. I.; Teng, X., Highly Active Iridium/Iridium-Tin/Tin Oxide Heterogeneous Nanoparticles as Alternative Electrocatalysts for the Ethanol Oxidation Reaction. *Journal Of The American Chemical Society* **2011**,133, 15172-15183.
288. Du, W.; Wang, Q.; LaScala, C. A.; Zhang, L.; Su, D.; Frenkel, A. I.; Mathur, V. K.; Teng, X., Ternary PtSnRh-SnO₂ nanoclusters: synthesis and electroactivity for ethanol oxidation fuel cell reaction. *Journal Of Materials Chemistry* **2011**,21, 8887-8892.
289. Du, W.; Su, D.; Wang, Q.; Frenkel, A. I.; Teng, X., Promotional Effects of Bismuth on the Formation of Platinum-Bismuth Nanowires Network and the Electrocatalytic Activity toward Ethanol Oxidation. *Crystal Growth & Design* **2011**,11, 594-599.
290. Danh, N.-T.; Frenkel, A. I.; Wang, J.; O'Brien, S.; Akins, D. L., Cobalt-polypyrrole-carbon black (Co-PPY-CB) electrocatalysts for the oxygen reduction reaction (ORR) in fuel cells: Composition and kinetic activity. *Applied Catalysis B-Environmental* **2011**,105, 50-60.
291. Alley, W. M.; Hamdemir, I. K.; Wang, Q.; Frenkel, A. I.; Li, L.; Yang, J. C.; Menard, L. D.; Nuzzo, R. G.; Ozkar, S.; Yih, K.; Johnson, K. A.; Finke, R. G., Industrial Ziegler-Type Hydrogenation Catalysts Made from Co(neodecanoate)(2) or Ni(2-ethylhexanoate)(2) and AlEt₃: Evidence for Nanoclusters and Sub-Nanocluster or Larger Ziegler-Nanocluster Based Catalysis. *Langmuir* **2011**,27, 6279-6294.
292. Iqbal, Z.; Patlolla, A.; Wang, Q.; Frenkel, A. I.; Zunino III, J. L.; Skelton, D. R., Studies of the blue to red phase transition in polydiacetylene nanocomposites and blends In *Mat. Res. Soc. Symp. Proc.*, 1190 Warrendale, PA, 2009; pp 1190-NN11-04.
293. Kossoy, A.; Frenkel, A. I.; Wang, Q.; Wachtel, E.; Lubomirsky, I., Local Structure and Strain-Induced Distortion in Ce_{0.8}Gd_{0.2}O_{1.9}. *Advanced Materials* **2010**,22, 1659-+.
294. Kossoy, A.; Frenkel, A. I.; Feldman, Y.; Wachtel, E.; Milner, A.; Lubomirsky, I., The origin of elastic anomalies in thin films of oxygen deficient ceria, CeO_{2-x}. *Solid State Ionics* **2010**,181, 1473-1477.
295. Qian, Q.; Tyson, T. A.; Deleon, M.; Kao, C. C.; Bai, J.; Frenkel, A. I., Influence of strain on the atomic and electronic structure of manganite films. *Journal of Physics and Chemistry of Solids* **2006**, 68, (3), 458-463.
296. Shanthakumar, P.; Balasubramanian, M.; Pease, D. M.; Frenkel, A. I.; Potrepka, D. M.; Kraizman, V.; Budnick, J. I.; Hines, W. A., X-ray study of the ferroelectric [Ba_{0.6}Sr_{0.4}](YTa)(0.03)Ti-0.94]O-3. *Physical Review B* **2006**, 74, 174103.
297. Zhu, Y.; Zheng, J. C.; Wu, L.; Frenkel, A. I.; Hanson, J.; Northrup, P.; Ku, W., Nanoscale disorder in CaCu₃Ti₄O₁₂: A new route to the enhanced dielectric response. *Physical Review Letters* **2007**, 99, 037602
298. Frenkel, A. I.; Pease, D. M.; Budnick, J. I.; Metcalf, P.; Stern, E. A.; Shanthakumar, P.; Huang, T., Strain-induced bond buckling and its role in insulating properties of Cr-doped V₂O₃. *Physical Review Letters* **2006**, 97, 195502.

299. Frenkel, A. I.; Pease, D. M.; Budnick, J. I.; Shanthakumar, P.; Huang, T., Application of glancing-emergent-angle fluorescence for polarized XAFS studies of single crystals. *Journal of Synchrotron Radiation* **2007**, 14, 272-275.
300. Allimi, B. S.; Alpay, S. P.; Goberman, D.; Huang, T.; Budnick, J. I.; Pease, D. M.; Frenkel, A. I., Growth of V₂O₃ thin films on a-plane (110) and c-plane (001) sapphire via pulsed laser deposition. *J. Mat. Research* **2007**, 22, 2825-2831.
301. Frenkel, A. I.; Ehre, D.; Lyahovitskaya, V.; Kanner, L.; Wachtel, E.; Lubomirsky, I., Origin of polarity in amorphous SrTiO₃. *Physical Review Letters* **2007**, 99, 215502.
302. Korshin, G. V.; Chang, H. S.; Frenkel, A. I.; Ferguson, J. F., Structural study of the incorporation of heavy metals into solid phase formed during the oxidation of EDTA by permanganate at high pH. *Environmental Science & Technology* **2007**, 41, (7), 2560-2565.
303. Nawani, P.; Desai, P.; Lundwall, M.; Gelfer, M. Y.; Hsiao, B. S.; Rafailovich, M.; Frenkel, A.; Tsou, A. H.; Gilman, J. W.; Khalid, S., Polymer nanocomposites based on transition metal ion modified organoclays. *Polymer* **2007**, 48, (3), 827-840.
304. Nawani, P.; Gelfer, M. Y.; Hsiao, B. S.; Frenkel, A.; Gilman, J. W.; Khalid, S., Surface modification of nanoclays by catalytically active transition metal ions. *Langmuir* **2007**, 23, (19), 9808-9815.
305. Pease, D. M.; Frenkel, A. I.; Shanthakumar, P.; Huang, T.; Balasubramanian, M.; Budnick, J. I.; Brewe, D.; Abitbol, N.; Odom, O., Performance and improved design of the log spiral of revolution monochromator *AIP Conf. Proc.* **2007**, 882, 902-904.
306. Sarkar, S. K.; Kababya, S.; Vega, S.; Cohen, H.; Woicik, J. C.; Frenkel, A. I.; Hodes, G., Effects of solution pH and surface chemistry on the postdeposition growth of chemical bath deposited PbSe nanocrystalline films. *Chemistry of Materials* **2007**, 19, (4), 879-888.
307. Si, M.; Zaitsev, V.; Goldman, M.; Frenkel, A. I.; Peiffer, D. G.; Weil, E.; Sokolov, J. C.; Rafailovich, M. H., Self-extinguishing polymer/organoclay nanocomposites. *Polymer Degradation and Stability* **2007**, 92, 86-93.
308. Solomon, A.; Akabayov, B.; Frenkel, A.; Milla, M. E.; Sagi, I., Key feature of the catalytic cycle of TNF- α converting enzyme involves communication between distal protein sites and the enzyme catalytic core. *Proceedings of the National Academy of Sciences of the United States of America* **2007**, 104, (12), 4931-4936.
309. A. I. Frenkel, Y. Feldman, V. Lyahovitskaya, E. Wachtel, I. Lubomirsky "Microscopic origin of polarity in quasi-amorphous BaTiO₃", *Phys. Rev. B* **2005**, 71, 024116.
310. A. V. Kolobov, P. Fons, A. I. Frenkel, A. Ankudinov, J. Tominaga, T. Uruga, "Understanding the phase-change mechanism of rewritable optical media", *Nature Materials* **2004**, 3, 703-708.
311. Kim, J.; Korshin, G. V.; Frenkel, A. I.; Velichenko A. B. "Electrochemical and EXAFS studies of effects of carbonate on the oxidation of arsenite" *Environ. Sci. Technol.*, **2006**, 40, 228-234.
312. O. Mabayoje, Y. Liu, M. Wang, A. Shoola, A. M. Ebrahim, A. I. Frenkel, C. B. Mullins *Electrodeposition of MoS_x hydrogen evolution catalysts from sulfur-rich precursors* *ACS Applied Mater. Interf.* **11**, 32879-32886 (2019)

