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Hydroxylamine decomposition on Cu(111) surface using Pynta

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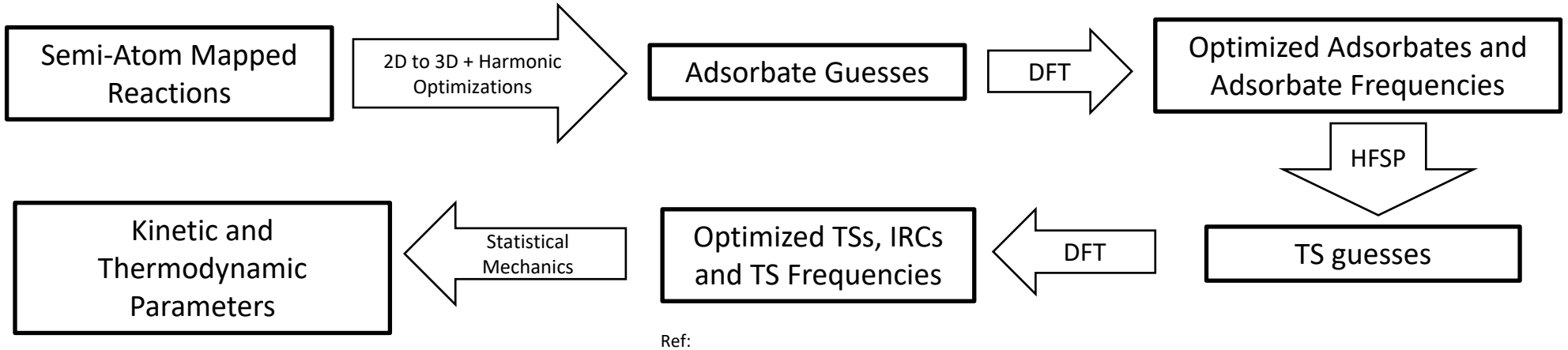
Pynta: An Automated Workflow for Calculation of Surface and Gas-Surface Kinetics

- Pynta (https://github.com/zadorlab/pynta) [1] is an automated workflow code for exploring reaction paths, which can automatically set up and spawn a large number of quantum chemistry calculations to study reactions of adsorbates and gas-phase species on metal facets.
  - Features:
    - Characterization of elementary chemical reaction mechanisms relevant to heterogeneous catalysis
    - Transition state guess using a novel technique "Harmonically forced saddle point searching"
    - Thermochemistry and rate coefficient calculations of surface and gas-surface reactions.
  - Workflow:
    - ASE[1] and Sella[2] are used to automate quantum chemistry calculations
    - The Fireworks[3] workflow management software is used to manage the calculations



Ref:
[1] Johnson, M.S., Gierada, M. Hermes, E.D., Bross D.B.., Sargsyan K., Najm, H.N, Zádor, J. ACS Spring 2023 National Meeting
[2] Hjorth Larsen, A. et al. *Journal of Physics: Condensed Matter*, *29*(27), 273002
[3] Hermes, E. D., Sargsyan, K., Najm, H. N., & Zádor, J. https://doi.org/10.1021/ACS.JCTC.2C00395
[4] Jain, A., et al. *Concurrency and Computation: Practice and Experience*, *27*(17), 5037–5059.

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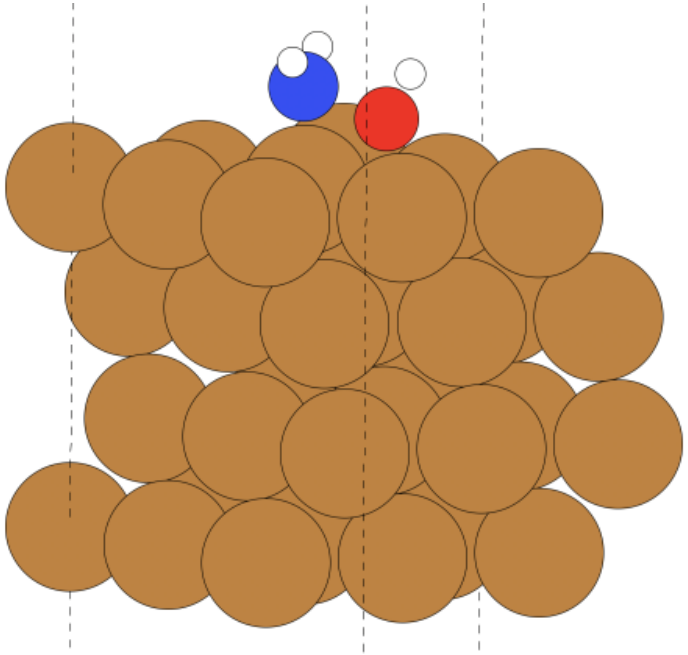
- Computational method to investigate ionic liquids + catalyst mechanisms
- Hydroxylamine (HA) decomposition on Cu(111) surface using Pynta
  - Goal:
    - To identify chemical mechanisms of catalytic decomposition of HA
    - To build microkinetic models for the catalytic decomposition reaction of HA
  - Background:
    - Hydroxyammonium nitrate (HAN) is a promising monopropellant thruster
    - HAN decomposes to HA, which is a primary product that further decomposes to create ignition conditions in HAN-based propellant
    - HA Catalytic decomposition products on various metal surfaces are not yet identified
  - Target:
    - Find accurate transition states and explore reaction pathway for HA decomposition reactions, which can possibly lead to various decomposition products
    - Calculate rate coefficients for identified reaction mechanisms
  - Reactions to investigate (One-step reactions): on fcc Cu(111) surface,

1. $H_2NOH \rightarrow NH_2 + OH$
2. $H_2NOH \rightarrow NH_2O + H$
3. $H_2NOH \rightarrow NHOH + H$

  - Further reaction pathways from above decomposition reactions will be investigated



Pynta estimated TS for reaction1.