SAND2020-2865PE

Revealing the Molecular Structure of Soot Precursors

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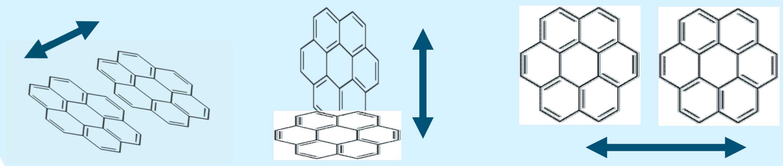
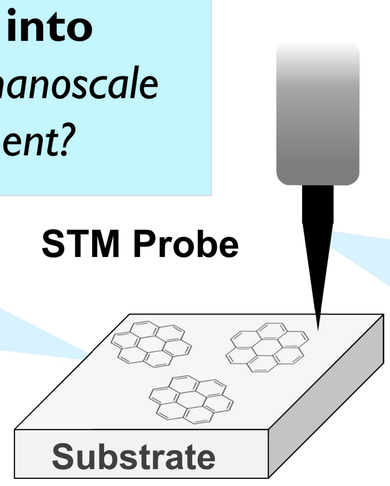
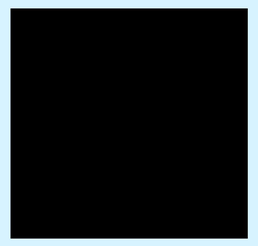
How do precursor molecules coalesce into incipient soot? *Can surface science reveal the nanoscale materials and physics that shape our environment?*

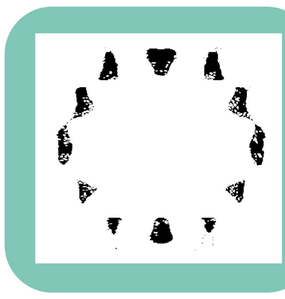
Intermolecular Interaction





Microscopy | **Simulation** | **Prior Theory**

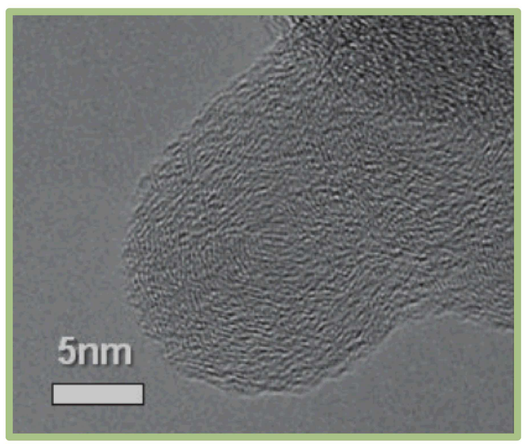




Compare

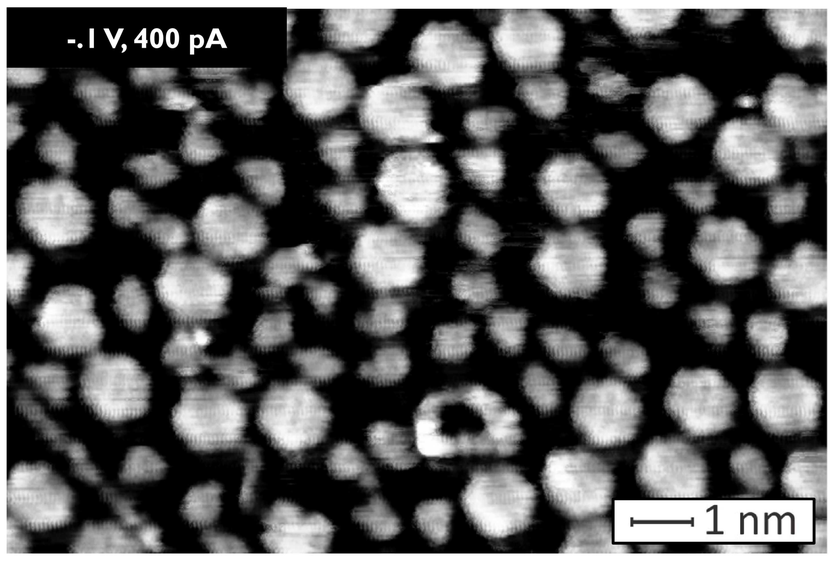
Combine Scanning Tunneling Microscopy and Density Functional Theory

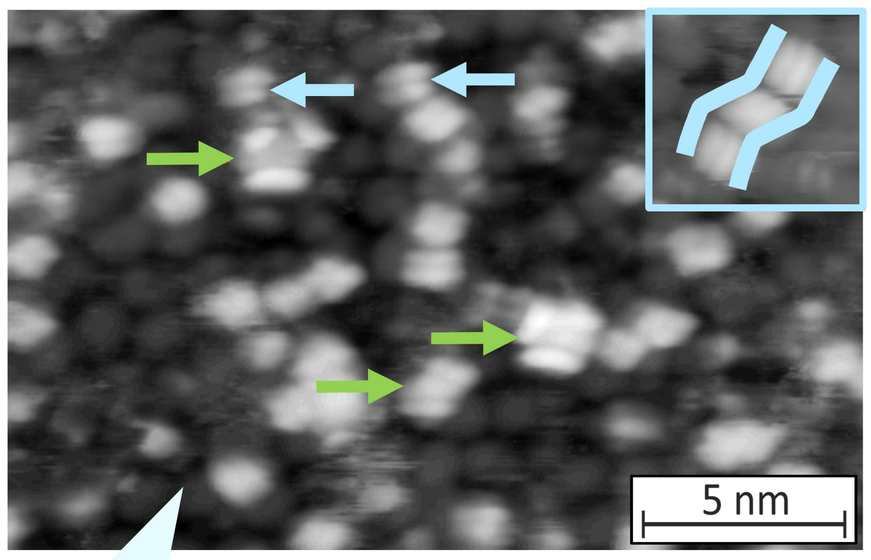
Goal: "grow" ~2nm nascent soot cluster that precedes a **primary particle** using the precursor species $C_{12}H_{24}$.



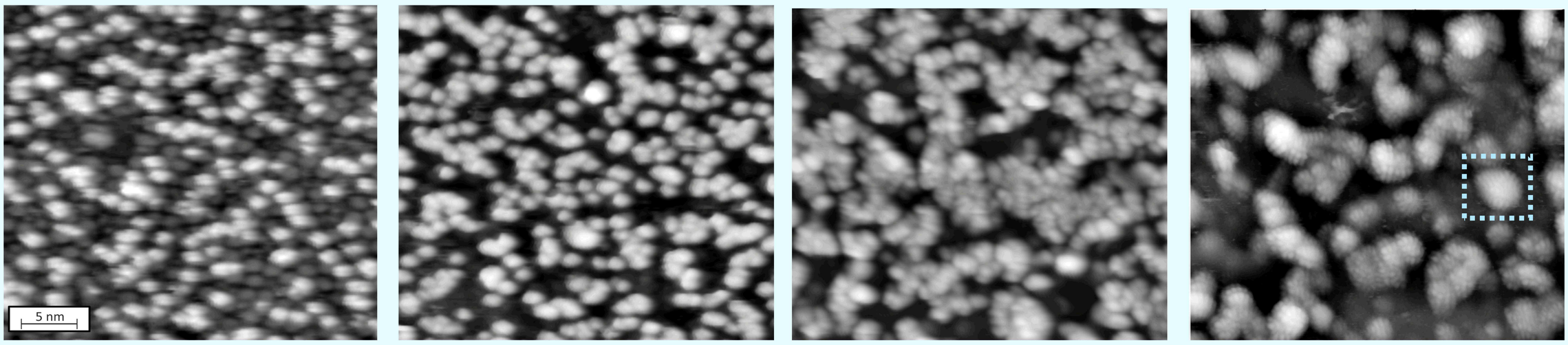
Miyashita et. al. SAE Tech. Paper 2015.

Deposit Increasing Amounts of Coronene on Pt





Anneal from Room Temperature to 600°C

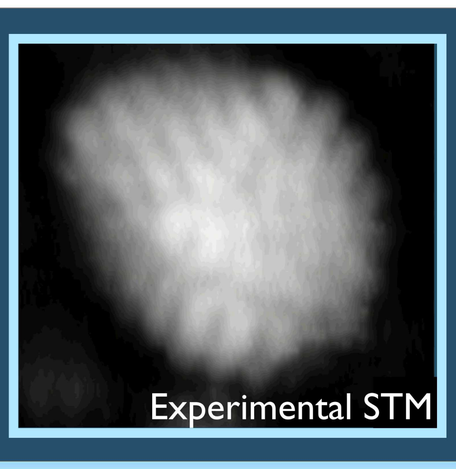


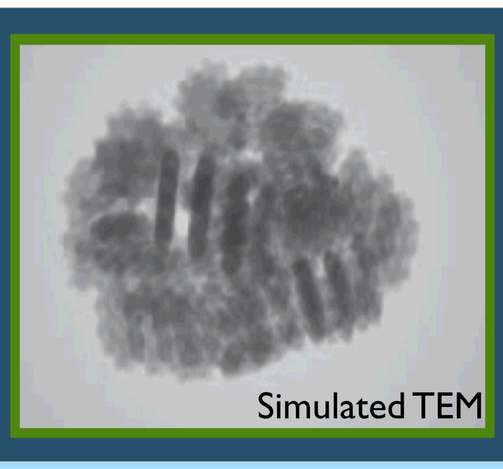
Molecules are *slightly offset and nearly parallel*, changing gradually throughout the cluster, matching **proposed theory.** (*Totton et. al. Combustion & Flame. 2010*)

Summary & Impact

This work presents **some of the most detailed experimental** information to date about the internal structure of incipient soot. Such fundamental data improves predictive combustion models and influences **next generation engine** design.

Soot research promotes **energy efficiency & pollution mitigation** in everyday combustion. More broadly, this work demonstrates the potential of surface science to unravel the **nanoscale materials & physics that effect the environment**.





Contributors & Collaborators: Scott Skeen and Regina Ragan

Wang, Bartelt, Ragan, Thürmer. Carbon. 129. 2018.

Wang, Thürmer, Skeen, Bartelt. In Prep.

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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