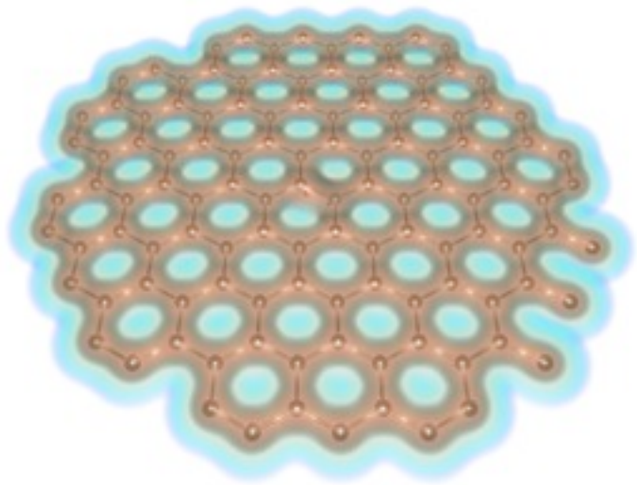

Uncertainty Classification of Molecular Interfaces

Aaron Knoll[1], Bin Liu[2], KC Lau[3], Maria Chan[2], Aslihan Sumer[4], Jeffrey Greeley[2], Larry Curtiss[3], Julius Jellinek[4], Mark Hereld[1] and Michael E. Papka[1]

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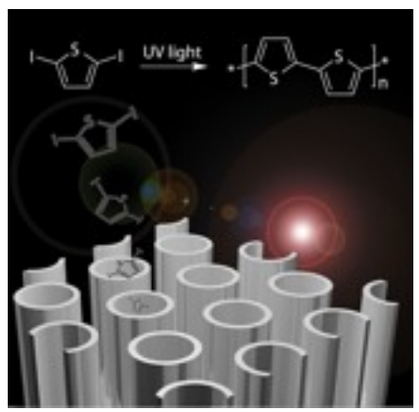
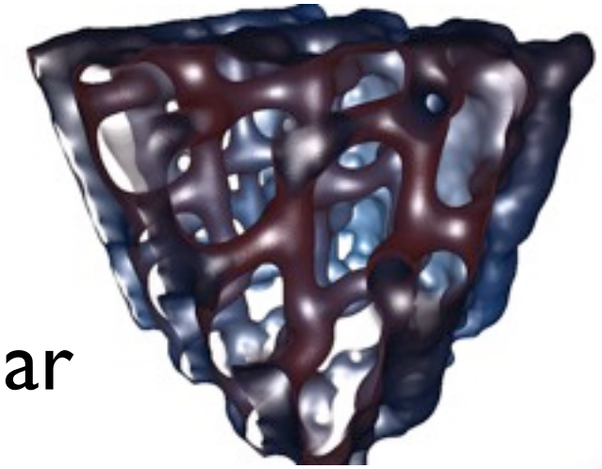
Argonne National Laboratory

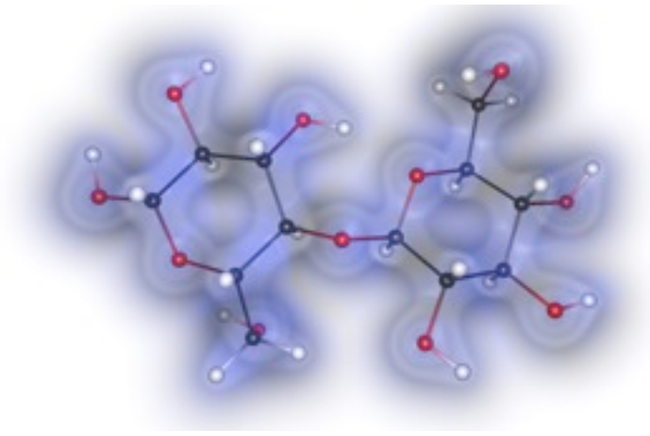
Motivation

- Computational chemistry drives **new energy science**.
- catalysis, diffusion, oxidation, heat/energy transfer, structure
- battery, photovoltaic, synthetic & biofuels, biomass conversion
- vis, analysis needed for MD, DFT
  - materials data have special needs.

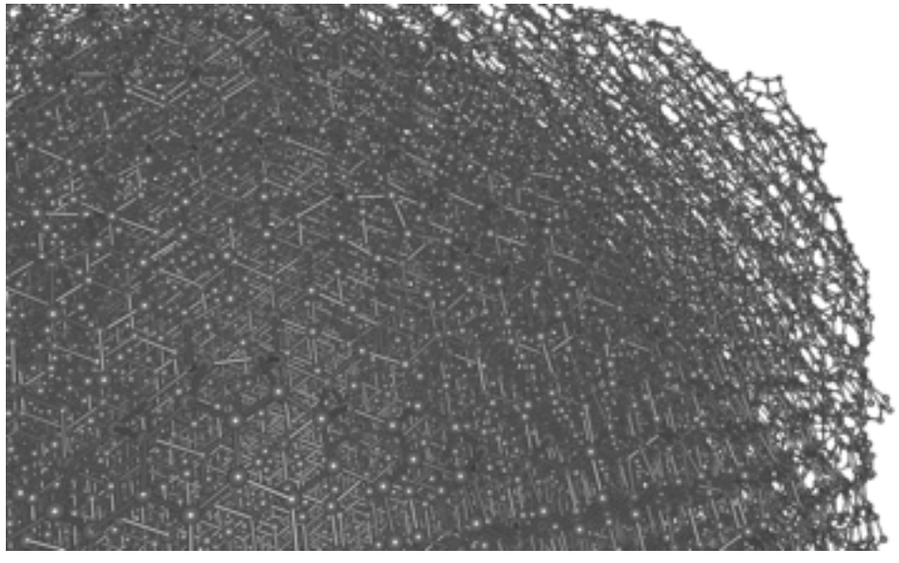


Challenges in molecular vis





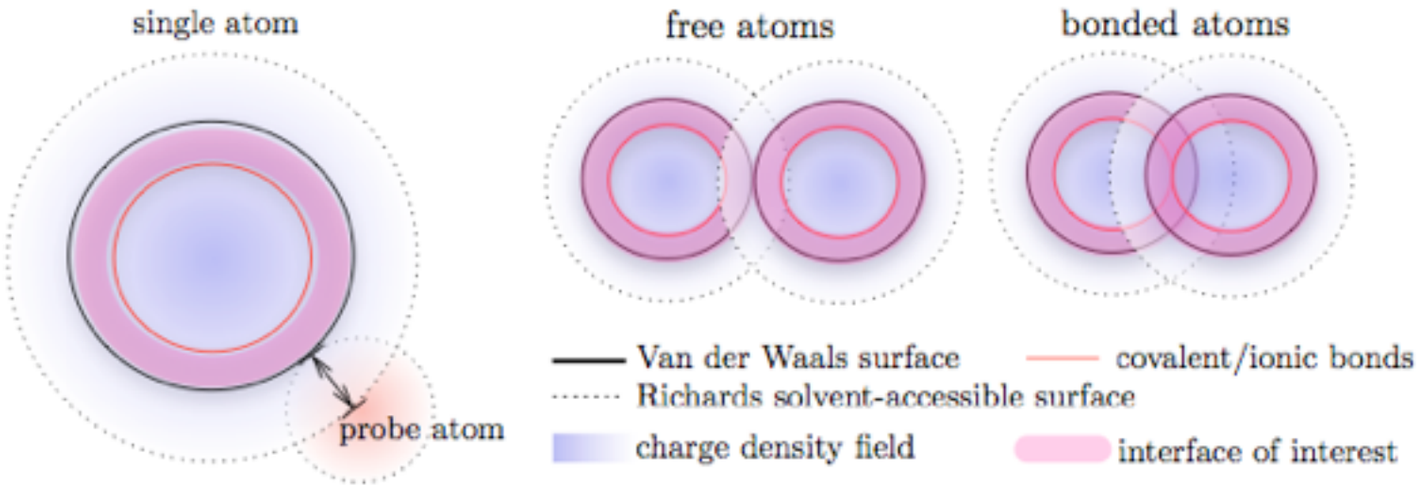
- How do we represent molecular surfaces?
- How do we interpret electron density fields computed from DFT?
- How do we visualize macromolecules?



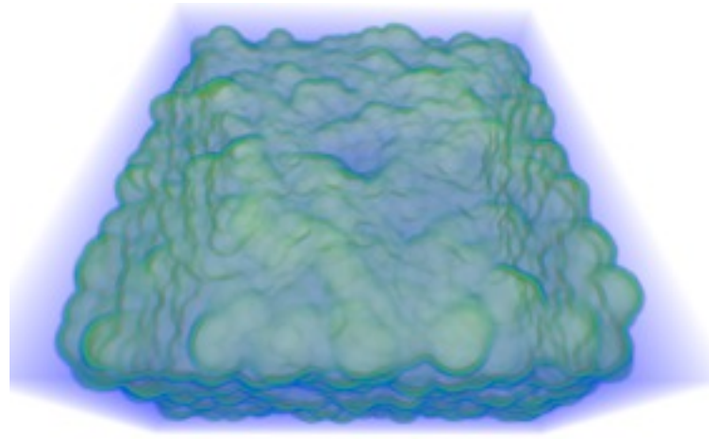
Scientific background

- Molecular structure is continuous:
  Self-consistent field (SCF) theory
  - Schroedinger Equation $E\psi = H\psi$
  - LCAO DFT $\theta_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$
- Density Functional Theory (**DFT**): simulate electrons
  - chemical bonds, activation energy
- Molecular Dynamics (**MD**): simulate atoms
  - intermolecular forces, heat, diffusion

Atomic radii

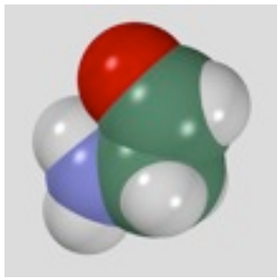


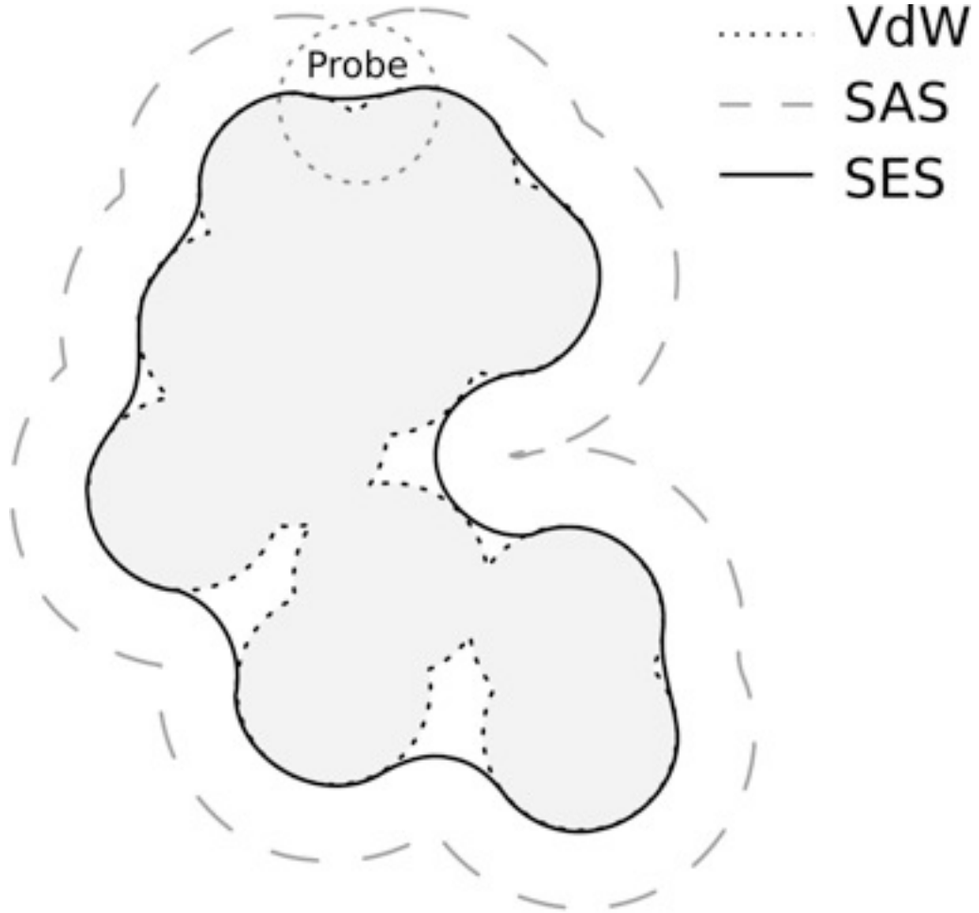
- Van der Waals radius = half the distance between *free* atoms.
- Chemical bond radii
  - covalent, ionic, metallic
- In practice, "surfaces" exist inside VDW radius

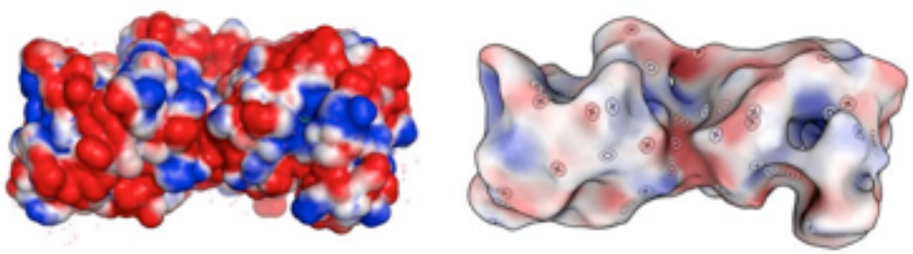


Molecular surfaces

- Van der Waals surface / CPK
- Richards 1971
- Connolly surfaces
  - Solvent-Accessible Surfaces
  - Solvent-Excluded Surfaces
- other abstractions, ribbons



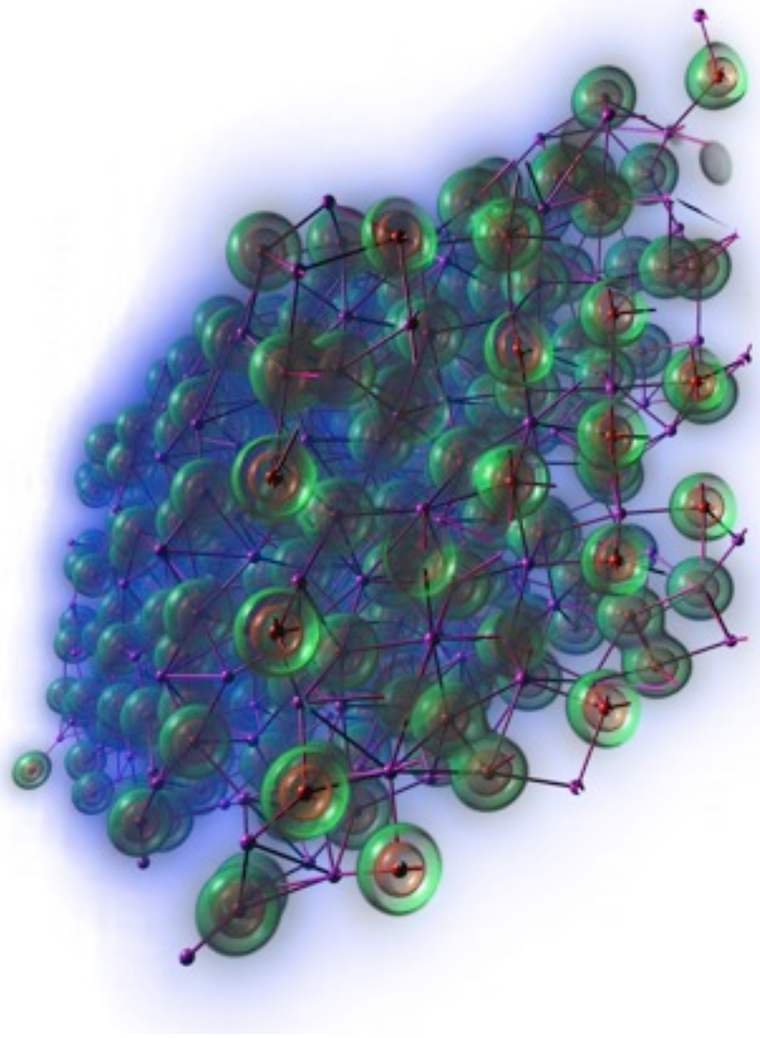




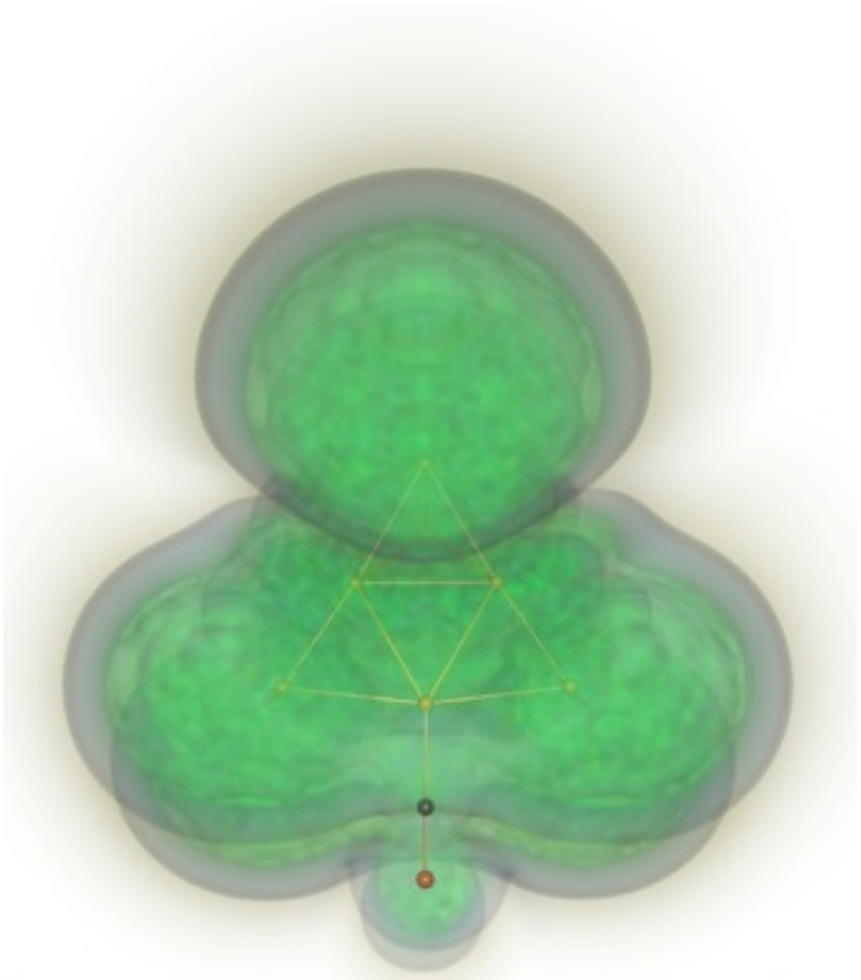
Cipriano & Gleicher, TVCG 07

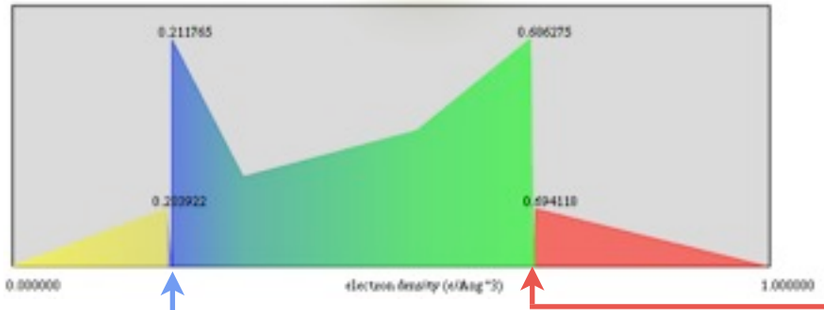
Nanovol

- Domain-specific vis tool
  - ball & stick
  - volume rendering from SCF or other fields
  - selection/modeling/analysis
- GPU ray-casting for interactive rendering
  - Tri-cubic spline interpolation
- Volume render electron density field (SCF)
  - generate approximate density field for larger MD data
  - feed transfer functions into analysis code



Uncertainty classification



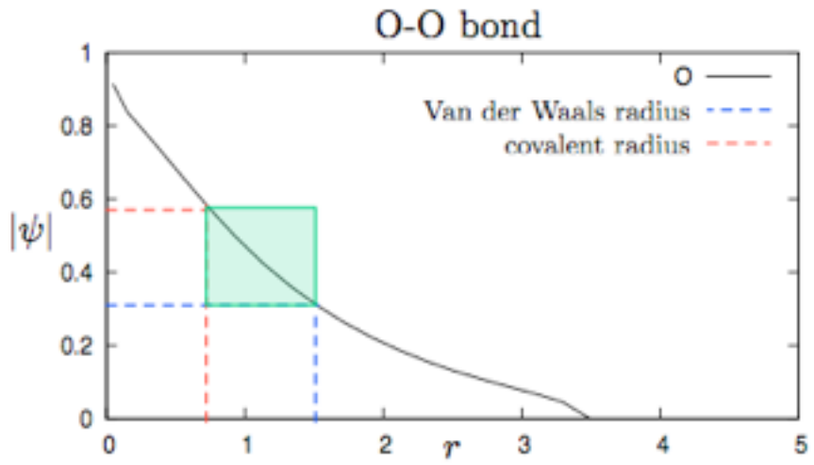


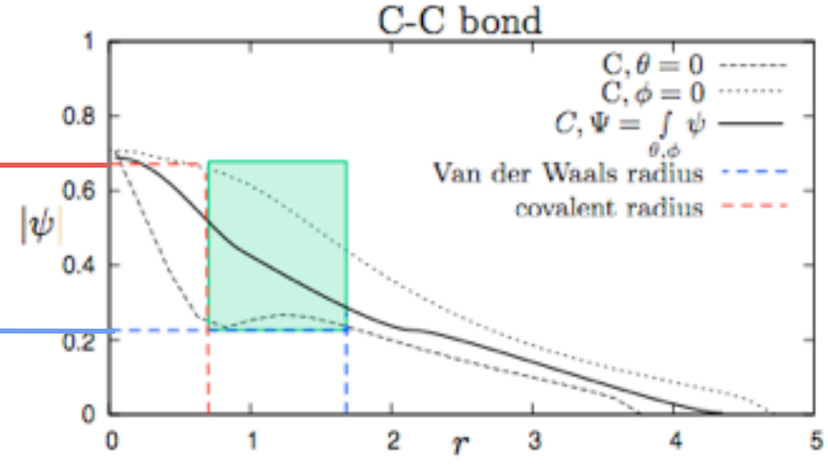
outside

interface
(we don't know)

inside

- Get distribution of abs(electron density) vs radius, from DFT on bulk compound
- Map Van der Waals, chemical bond radii to a **density interval.**
  - use this in a transfer function.



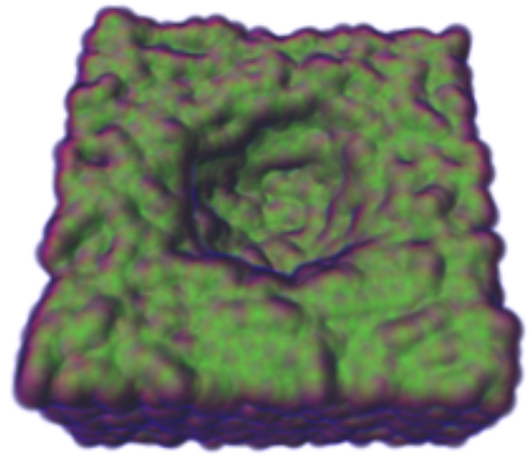


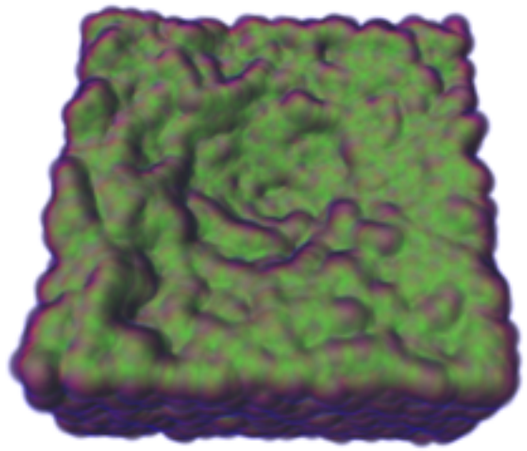
DFT use case: CO Adsorbtion

- DFT computation in NWChem
- bonding energetics of CO in Pt_7 cluster
- White: made-up (*ad hoc*)
- Gold: metallic radius of Pt (in Pt-Pt)
- Green: covalent bond of C (sp^2 dimer)
- Blue: Van der Waals radius of C

Approximate density fields

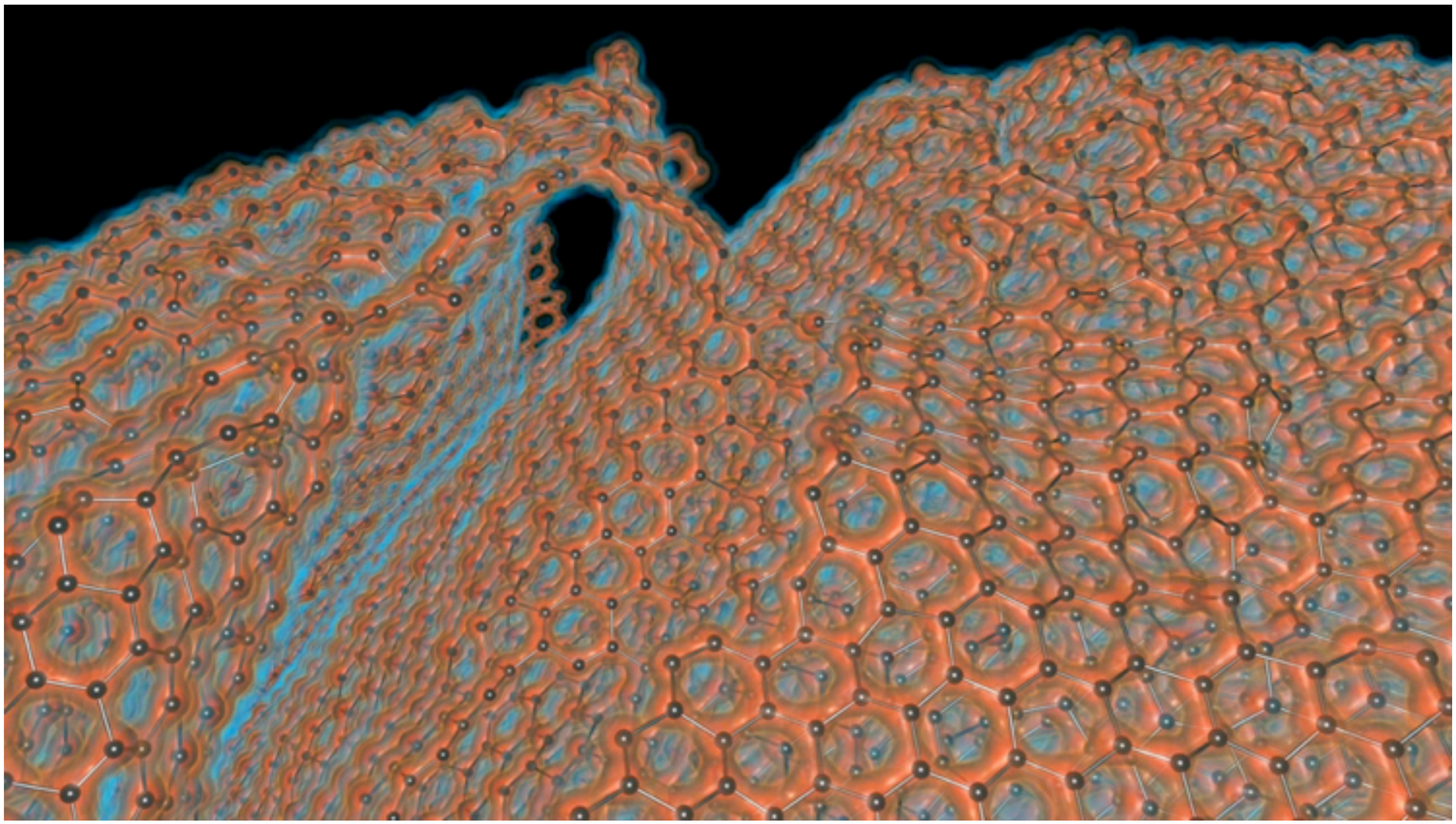
- Create a good approximation of electron density for larger molecules
- Use distribution from DFT data to model electron density for individual atoms
  - linear combination of *atomic* basis functions $|\psi| = \sqrt{\rho}$ $r_i(\vec{x}) = |\vec{x} - \vec{p}_i|$ $\Psi(\vec{x}) = \sum_i \Theta_i(r_i(\vec{x}))$
- Computation is fast, trivial to parallelize





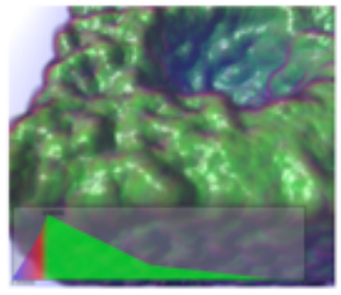
MD use case: supersoot

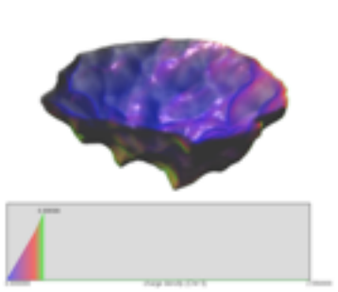
- amorphous carbon, 740k atoms, MD computation of thermal annealing in LAMMPS
- Show bond structure even at a distance
- Find possible Lithium diffusion paths

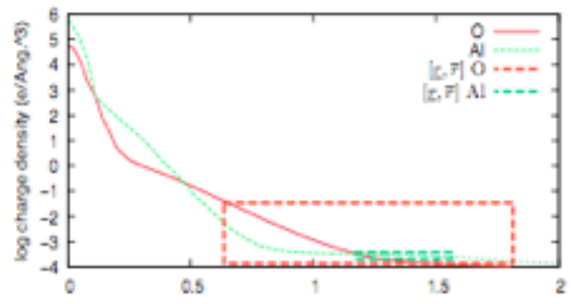


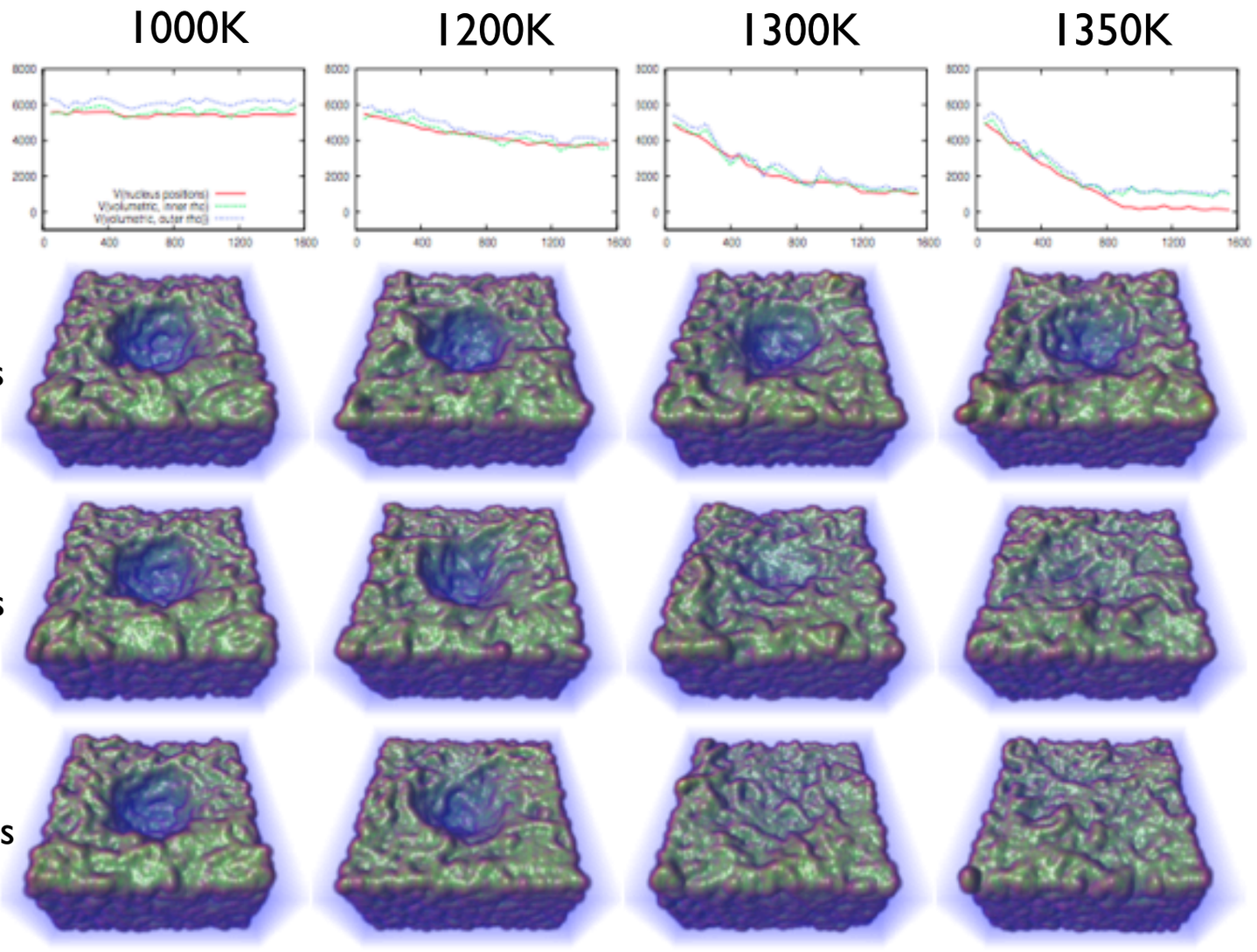
MD use case: nanobowls

- alumina oxide nanobowls, 20k atoms x 150,000 timesteps in DL_POLY
- Use density volume, uncertainty classification to perform geometric analysis
  - bowl volume
  - surface area
  - curvature
- meaningful upper/lower bounds
- WYSIWYG



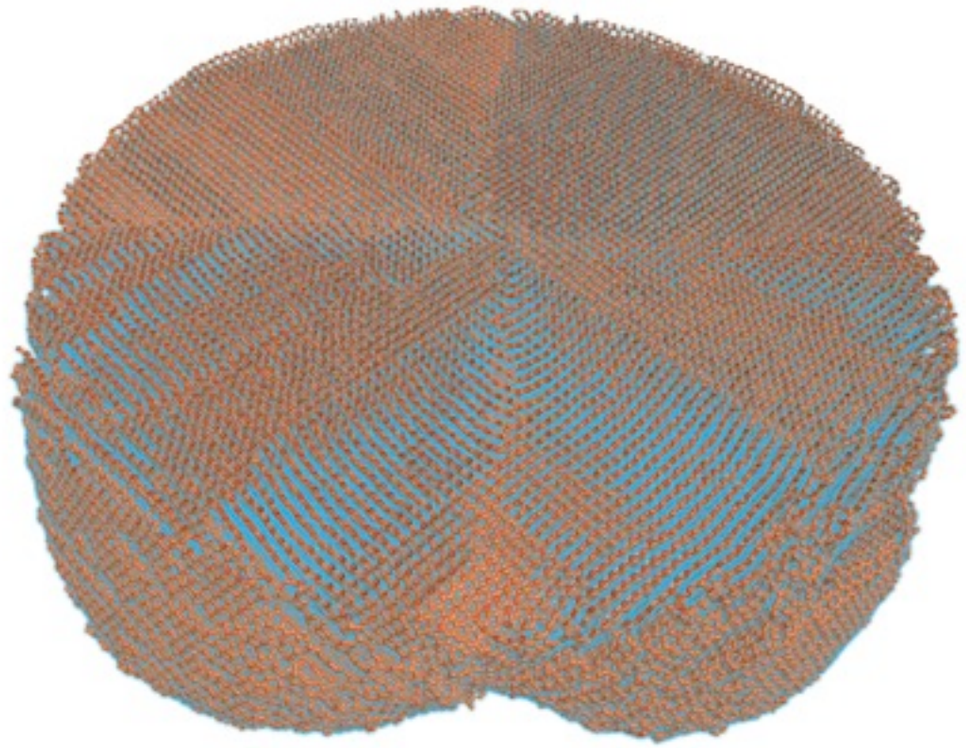


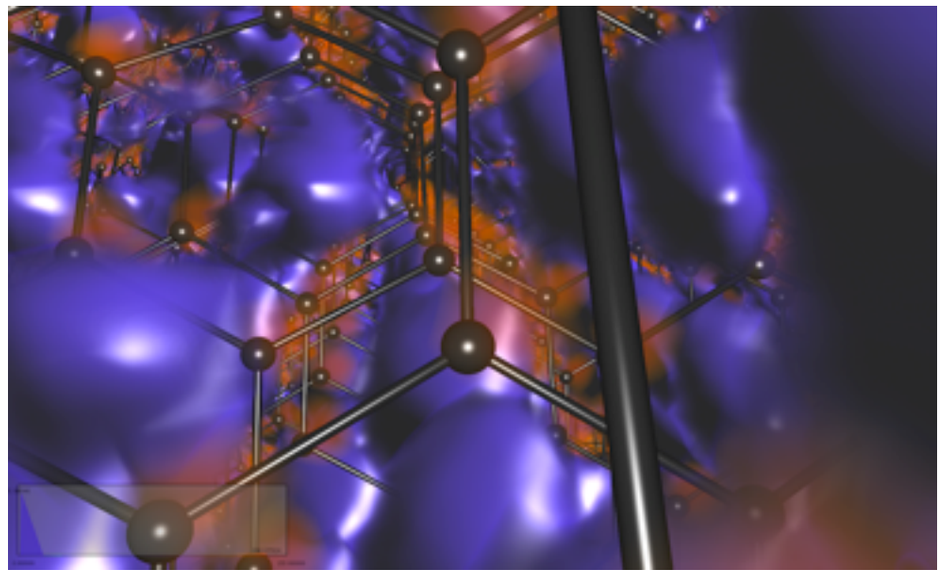




Conclusions

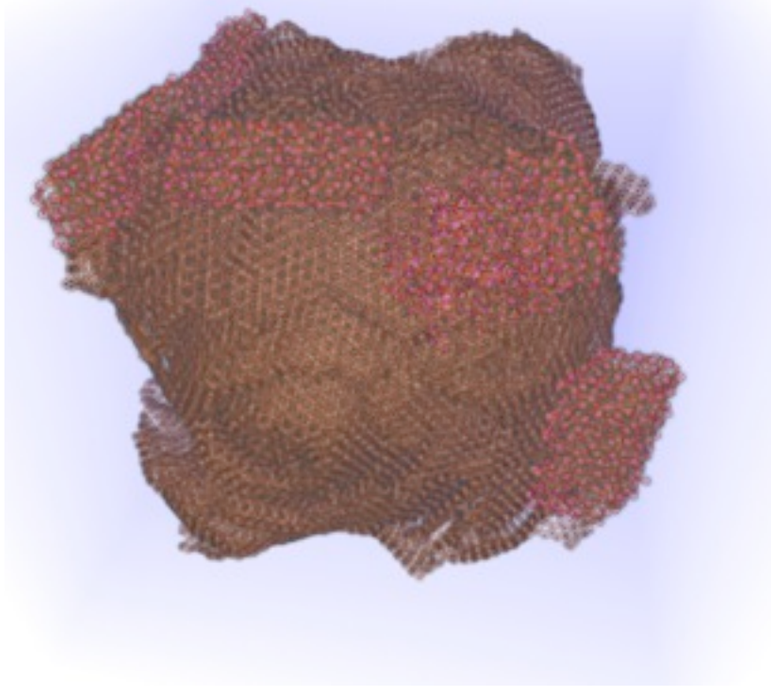
- volume vis has potential in chem/materials applications
- Our contributions:
  - classify according to physically relevant electron density isovalues
    - inside, outside, and “we don’t know”!
    - molecular interfaces with uncertainty
  - use distribution to model approximate electron density

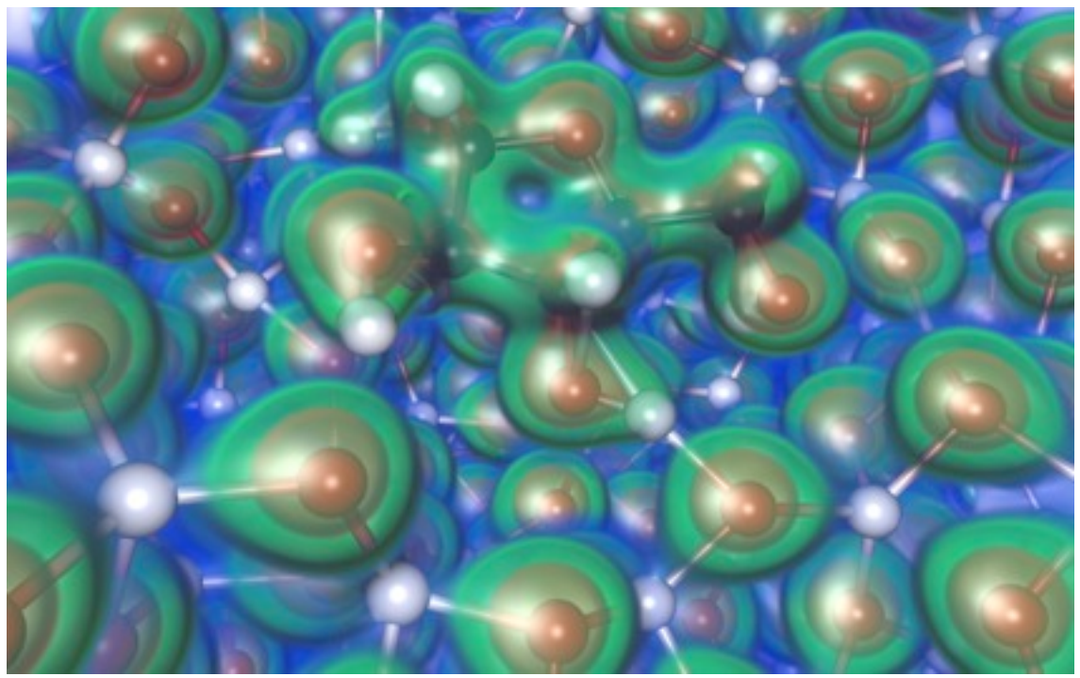


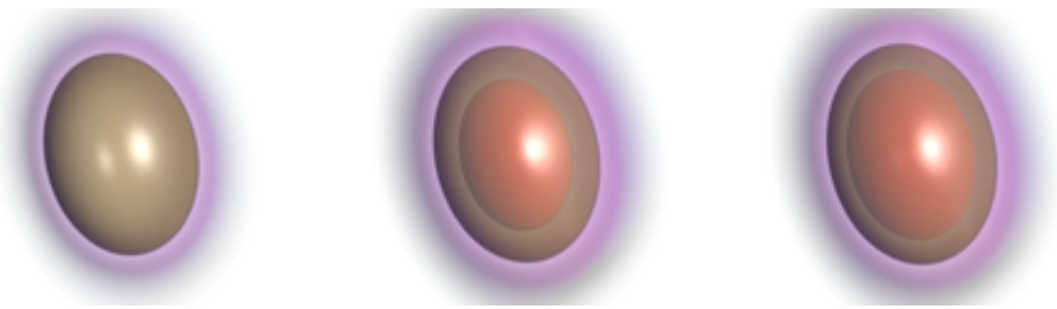


Future work

- Expose these capabilities to more scientists
  - actually use scalar field data from DFT!
  - explore mesascale phenomena in MD
- Classify electrostatic potential
- Classify using multiple distributions
- Similar applications (nuclear DFT)?







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