Surface Studies with Combined Free Energy Functionals of Electronic and Liquid Densities

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Free Energy Functionals for Solvated Surfaces

Solvated Surfaces: Potential Applications
- Catalysis
- Surface Stability

Which Solvation Theory is Appropriate?

![Diagram showing various solvation theories and their applications]

Joint Density-Functional Theory (JDFT)
Rigorous description of electronic systems in complex environments
- Solvent Electron Density:
  - Solvent atom densities
  - Electronic density fluctuations

Liquid Functional

![Diagram showing liquid functional representation]

Density-Only DFT: Thomas-Fermi-LDA approximation

Coupling Functional

![Diagram showing coupling functional representation]

Double Layer and Adsorption Capacitance

Metal Surfaces in Aqueous Electrolyte

Gouy-Chapman-Stern Model
- Structure of the double layer in terms of spacing and orientation
- Saturation of the dielectric in strong fields
- Differences in ionic and electronic states
- Ion-ion correlation

Voltage-Dependent Structure

Potential of Zero Charge (PZC) from vacuum to solvated surface

Double Layer and Adsorption Capacitance

Rutile TiO₂ (001) in Water

![Diagram showing Rutile TiO₂ (001) in Water]

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