Thermodynamic Integration Simulation Method for Filling Molecular Enclosures Using Spliced Soft-Core Interaction Potential

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ABSTRACT

Researchers have developed a simulation method to determine the properties of molecular enclosures based on slow growth thermodynamic integration (SGTI).

FULL DESCRIPTION

Molecular enclosures appear often in both solid-state materials and biological systems, including nanoporous materials for energy storage and nanolipid particles for drug delivery. The constituent ions and molecules within these enclosures can largely determine the properties and performance of the entire system. Therefore, it is critical to determine their density, relative concentration, arrangement, physical and electronic structure, viscosity, diffusivity, and other properties. However, these properties can vary dramatically, yet often remain poorly understood. So improving understanding of how these systems are assembled can improve their design and efficacy in a variety of applications.

Working together, researchers at the University of California, Davis and collaborators at Lawrence Livermore National Laboratory have developed a simulation method based on SGTI that improves understanding of the properties of molecular enclosures. SGTI is an improvement compared to standard thermodynamic integration (TI), because SGTI only requires knowledge of the initial state, while TI requires knowledge of states along the entire integration. The SGTI method developed employs a spliced soft-core interaction potential (SSCP) that is designed to more accurately represent the target hard-core interaction potential (HCP). The proposed method allows proper wall thickness to be maintained when filling an enclosure, an important consideration when attempting to maintain the target thickness of the enclosure's wall. The proposed SSCP can be used in any system employing a standard soft[core potential (SCP), and should be tunable to outperform previously-used SCPs in a wide variety of applications.

APPLICATIONS

- Increase fidelity of simulations
- Helps determine the properties of molecular enclosures
- Can be incorporated into many standard simulation packages
- Important for any system in which the size of the constituent contents (e.g., ions, molecules, polymers) is commensurate with wall thickness and final enclosed volume of the enclosure

FEATURES/BENEFITS

- More accurate than previously used techniques
- Only requires knowledge of initial state of the system

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OTHER INFORMATION

KEYWORDS

Carbon nanotube, Molecular dynamics, Simulation, Soft-core, Thermodynamic integration

CATEGORIZED AS

- **Computer**
  - Other
- **Energy**
  - Other
  - Storage/Battery
- **Materials & Chemicals**
  - Nanomaterials
  - Storage
  - Superconductors
- **Medical**

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Issued Patent	11,734,478	08/22/2023	2019-572

Additional Patent Pending

- Delivery Systems
- Other
- Research Tools

RELATED CASES

2019-572-0

ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

- Biomimetic Chemical Compounds for Capturing Carbon Dioxide from Power Plant Stacks and the Atmosphere

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