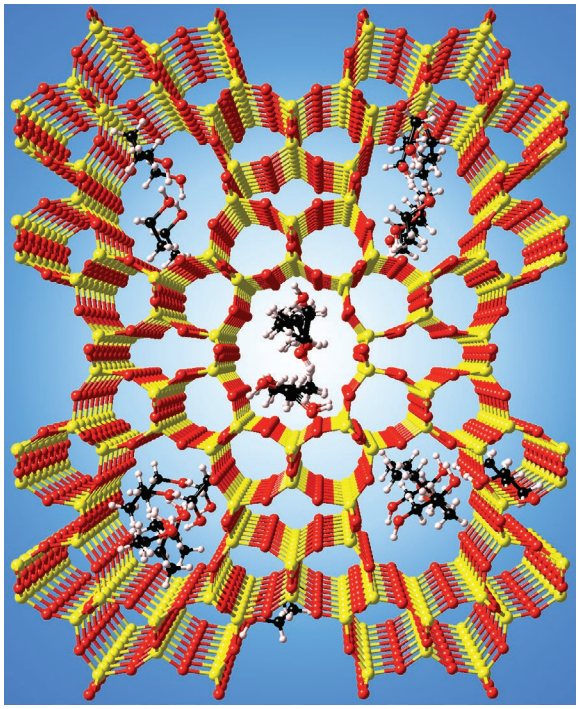
materials design®

MedeA® Docking

MedeA® Docking automatically creates, manipulates and refines host-guest systems. Employing the well known Metropolis Monte Carlo algorithm[1], MedeA® Docking rapidly evaluates van der Waals interactions to generate and assess stable system configurations. The resulting host-guest structures are then usable in forcefield and first-principles based simulations. MedeA® Docking may be invoked interactively within the MedeA® environment or using MedeA® Flowcharts on the JobServer.

Key Benefits of MedeA® Docking:

- *Accelerates model construction and refinement*
- *Enables automated MedeA® Flowchart based model construction and screening*
- *Provides models for subsequent forcefield and first-principles based simulation*



A model of ethanol in Theta-1 generated using MedeA® Docking.

Key Features of MedeA® Docking:

- *Automatic combination of host and guest structures for screening and simulation*
- *Assessment of steric interactions*
- *Automated energy based refinement of sorbate position and orientation*
- *Interactive screen updates and full user control of model view and scale during docking*
- *Control of simulation length, Monte Carlo temperature, maximum displacements and rotation*
- *Combination of multiple sorbates with host structure*
- *Employs Metropolis Monte Carlo algorithm, allowing user control of the level of searching employed (through control of acceptance probability via the temperature setting)*
- *For use with surface, microporous and porous materials model*

Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® JobServer and TaskServer*

Supported MedeA® Modules

- *MedeA® LAMMPS*
- *MedeA® VASP*

[1] Metropolis, N.; Rosenbluth, A.W.; Rosenbluth, M.N.; Teller, A.H.; Teller, E. (1953). "Equations of State Calculations by Fast Computing Machines" J. Chem. Phys. 21, 1087–1092.

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