MedeA Docking

At-a-Glance

MedeA ®[1] *Docking* automatically creates, adjusts, and refines host-guest and surface-guest systems. Employing the well-known Metropolis Monte Carlo algorithm[2], *MedeA Docking* evaluates van der Waals interactions to generate and assess stable system configurations. The resulting host-guest structures may then be employed in forcefield and first-principles based simulations. *MedeA Docking* can be invoked interactively within the *MedeA Environment* or by using *MedeA Flowcharts* on the JobServer. *MedeA Docking* is a building tool that allows you to combine systems automatically to create the starting points for further simulation studies.

Key Benefits

- Saves time through accelerated and automated model construction and refinement
- Simplifies automated Flowchart based model construction for screening, allowing construction of host-guest and surface-guest systems without interactive manipulation
- Explores multiple guest configurations, searching and evaluating many possible binding configurations

Key Features

- Automatic combination of host and guest structures
- Minimization of steric overlap between host and guest
- Automated energy based refinement of sorbate position and orientation

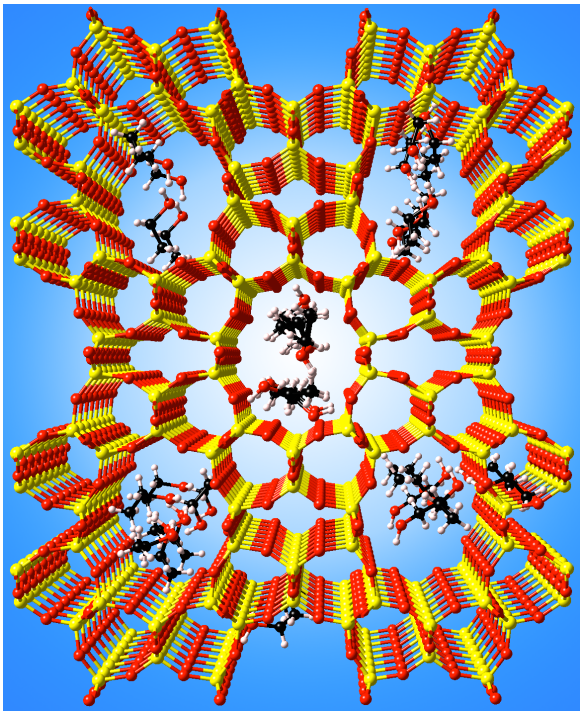

Figure 1: Alcohol molecules docked in a microporous material using MedeA Docking.

- Interactive screen updates, and full user control of model view and scale during docking
- Control of simulation length, Monte Carlo temperature, maximum position, and rotation displacements
- Combination of multiple sorbates with host structure
- Employs Metropolis Monte Carlo Algorithm, allowing user control of the employed search (via control of acceptance probability within the temperature setting)
- For use with surface, microporous, and porous materials models

'I will say that enzyme and glucoside must fit together like lock and key in order to be able to exercise a chemical action on each other'

Emil Fischer, 1852-1919

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

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

Required Modules

- *MedeA Environment*
- *MedeA JobServer and MedeA TaskServer*

Related Modules

- *MedeA LAMMPS*
- *MedeA VASP*
- *MedeA MOPAC*
- *MedeA Gibbs*
- *MedeA Gaussian GUI*

Find Out More

To learn more about the use of docking to provide insights into host-guest interactions in materials science, see the following papers on the following topics:

- General host-guest interactions[3],
- Understanding templating with organic additives[4],
- Simulating CFC interactions[5], and host-guest
- Interactions in isomerization[6].

Watch this webinar to learn more about atomistic simulation using the *MedeA Environment*:

- Explore the MedeA 2.22 atomistic simulation environment

[3] C.R.A. Catlow, J.M. Thomas, C.M. Freeman, P.W. Wright, R.G. Bell, "Simulating and predicting crystal structures", *Proc. R. Soc. Lond. A* **442**, 85 (1993)

[4] D.W. Lewis, C.M. Freeman, C.R.A. Catlow, "Predicting the templating ability of organic additives for the synthesis of microporous materials", *J. Phys. Chem.* **99**, 11194 (1995)

[5] A.R. George, C.M. Freeman, C.R.A. Catlow, "A computational investigation of zeolite-chlorofluorocarbon interactions" *Zeolites* **17**, 466 (1996)

[6] P.T. Tschaufeser, C.M. Freeman, "Computer simulation studies of the selectivity of zeolites for different butene isomers" *Catal Lett.* **60**, 77 (1999)

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