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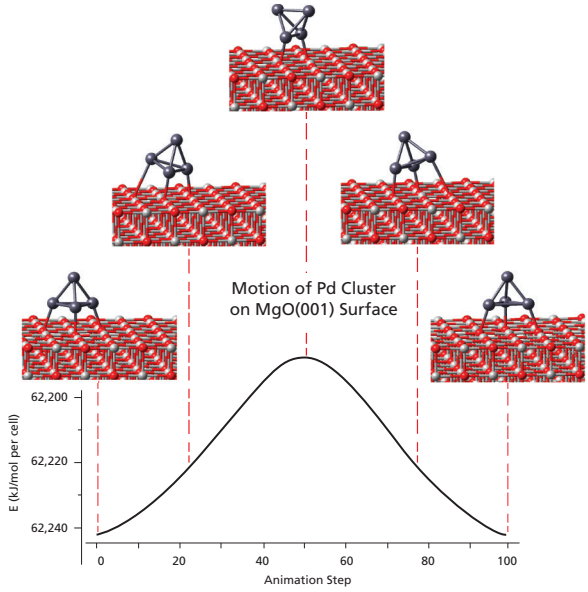
MedeA® Transition State Search

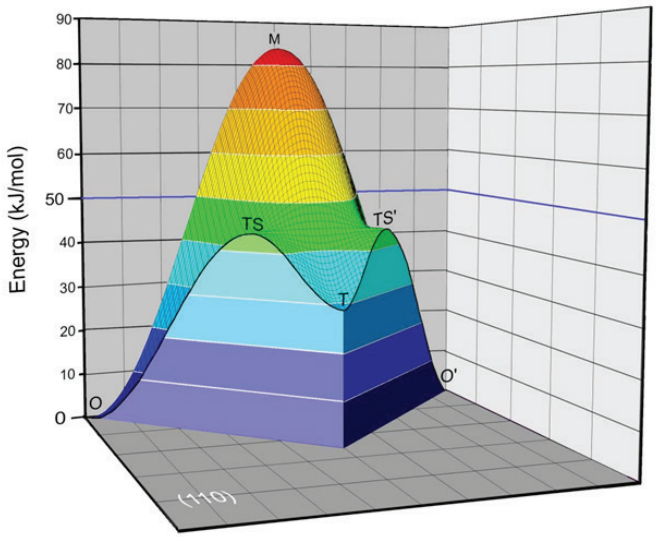
MedeA® Transition State Search determines the structure and energy of transition states in chemical reactions such as the dissociation of a molecule on a surface or the location and height of energy barriers in a diffusion process. Combined with the Phonon module, this allows the computation of reaction rates and jump rates as a function of temperature.

Transition states are saddle points in the potential energy surface of chemical systems; the connections between key regions of the potential energy hypersurface. Transition states determine system properties such as reaction rates and activation energy barriers, which govern kinetic and diffusive behavior. Given the importance of such properties, efficiently locating transition states is of considerable interest.

Mathematically, although a transition state is a stationary point (that is, the first derivative of the potential energy with respect to defined structural ordinates is zero); a single second derivative of the potential energy is negative, so in one particular direction the desired configuration is a local maximum of the potential energy surface. Locating such positions is computationally demanding as it is not a simple minimization problem. However, MedeA® Transition State Search makes the location of such transition states computationally efficient.



Application of the MedeA® Transition State Search module to the migration of a Pd_4 cluster on a MgO(001) surface.



A 3D rendering of the energy surface for hydrogen migration in Ni based on data obtained from MedeA® Transition State Search. Transition states between octahedral and tetrahedral sites within the lattice are labeled TS and TS'. See reference [3] for additional information.

MedeA® Transition State Search provides direct access to the Nudged Elastic Band (NEB) method [1,2]. The pathway connecting the initial and final configurations is explored at discrete intervals using a restraining force which keeps each configuration perpendicular to and regularly spaced along the connecting direction. Subject to these constraints, the highest of any obtained configuration provides a good initial estimate of the transition state between the supplied initial and final configurations.

Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® Environment Job and Task Servers*
- *MedeA®-VASP*

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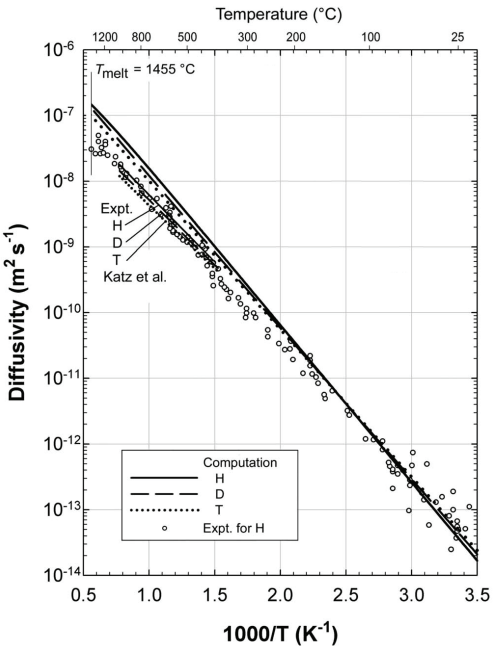
An illustration of the level of accuracy which may be obtained with MedeA® Transition State Search is provided in the figure below. The graph shows the computed diffusion coefficient for hydrogen in Ni as a function of temperature obtained through DFT calculations using MedeA® Transition State Search, MedeA®-Phonon and activated transition state theory as described in [3].



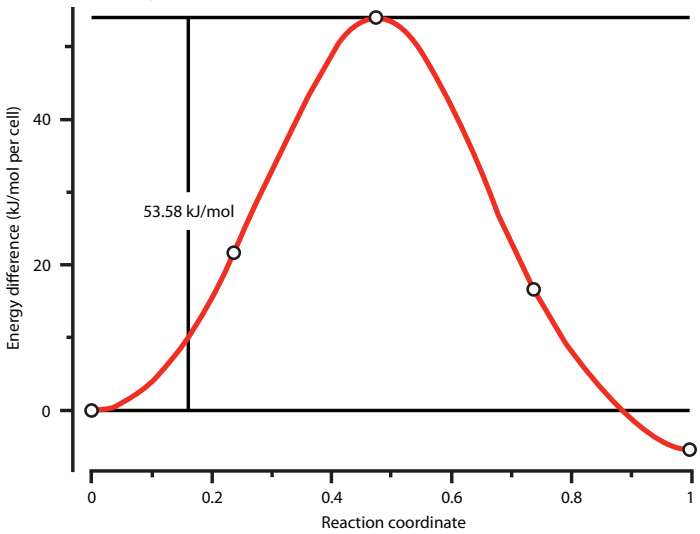
The computed diffusion coefficient is represented by the solid line and available experimental results by individual points. Clearly the agreement between experiment and computation is excellent illustrating what can be achieved with modern first-principles methods in combination with efficient transition state search capabilities.

References

[1] H. Jónsson, G. Mills, K.W. Jacobsen, in Classical and Quantum Dynamics in Condensed Phase Simulations Eds. B.J. Berne, G. Ciccotti and D. F. Coker (World Scientific), 385 (1998).

[2] G. Henkelman, B. Uberuaga, H. Jónsson, J. Chem. Phys. **113**, 9901 (2000).

[3] E. Wimmer, W. Wolf, J. Sticht, P. Saxe, R. Najafabadi, and G.A. Young Jr, Phys. Rev. B **77**, 34305 (2008).



Energy Profile for the diffusion of an oxygen atom on a Ni(111) surface from an hcp to an fcc site. An interactive slider provides accurate energy differences between any two points along the path.

Properties from MedeA® Transition State Search

- *Energy Profile Along Reaction Path*
- *Structure and Energy of Transition States*
- *Multiple Minima and Transition States*
- *Animation of Reaction Path*

Computational Characteristics

- *Fully integrated with the MedeA® environment Job and Task server infrastructure. Hence, computational resources may be efficiently employed in locating transition states.*
- *Nudged Elastic Band (NEB) Method*
- *Climbing Image Method*
- *BFGS2 Optimizer*
- *Automatic Refinement: automatic zoom on the region near the transition state thereby providing a new set of images*
- *Final Optimization Using Gradient Minimization*
- *Choice of any Number of Intermediate Images*

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