

# Transition State Search (TSS)

The TSS module determines the structure and transition state energy in chemical reactions such as the dissociation of a molecule on a surface or the location and barrier height in a diffusion process. Combined with the Phonon module this allows the computation of reaction and jump rates as a function of temperature.



Energy profile for the diffusion of an oxygen atom on a Ni(111) surface from an hcp to an fcc site hcp to an fcc site.

## **Properties from TSS module**

- Energy profile along reaction path
- Structure and energy of transition states
- Multiple minima and transition states
- Animation of reaction path

#### **Computational characteristics**

- Nudged elastic band method
- Climbing image method
- BFGS2 optimizer
- Automatic refinement (i.e. automatic zoom on region near transition state with new set of images)
- Final optimization using gradient minimization
- Choice of any number of intermediate images

#### **Required MedeA modules**

- Core MedeA environment
- MedeA VASP 4.6 or 5.2
- Job Server and Task Servers

### More on our website:

### www.materialsdesign.com

Diffusion of Hydrogen in Nickel

#### **Relevant Publications**

E Wimmer, W Wolf, J Sticht, P Saxe, R Najafabadi, and G Young, *Physical Review B Condensed Matter* vol. 77 p. 134305, 2008