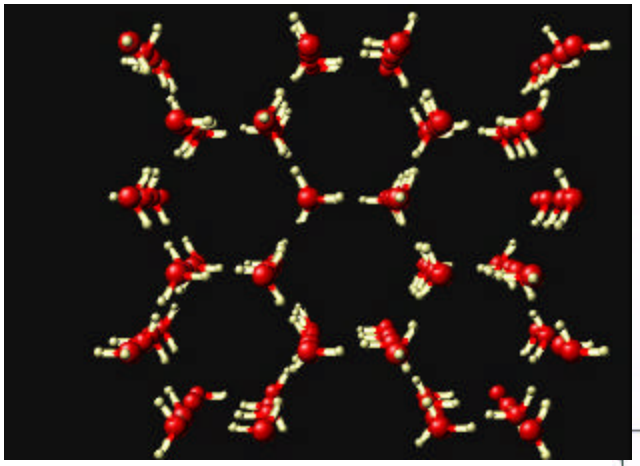
Pilot-CSD5 Highlight

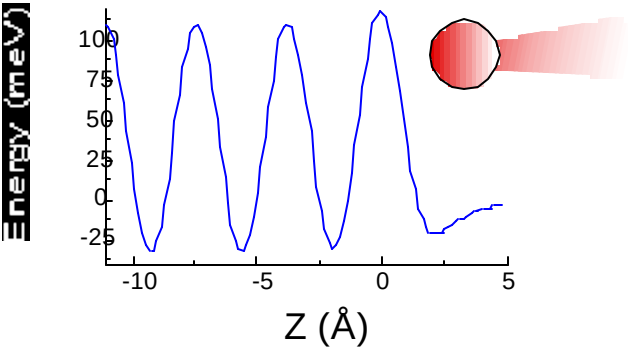
Project: He Scattering on Cubic Ice and ASW

EMSL

Model Ice Surface

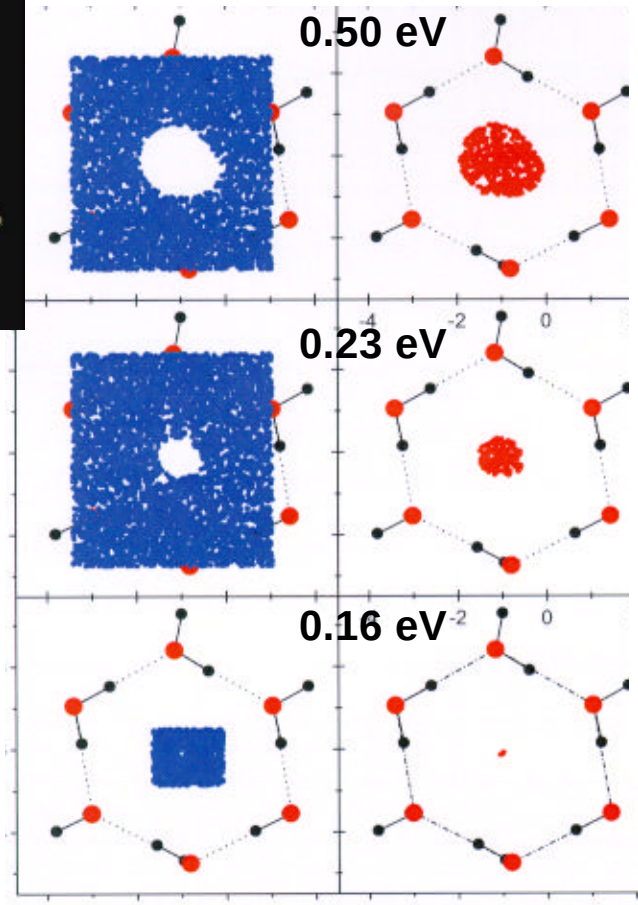


Model Ice Potential Energy surface



Classical Trajectories of He / Ice Absorption

Reflected He Absorbed He



Fundamental Aspects of the Dynamics of Gas/ Ice Surface Interaction

The interactions of gas phase molecules with the ice surface is an important aspect of the overall chemical reactivity that occurs on ice particles in the atmosphere. Many factors influence these interactions including pressure, temperature and structure of the ice surface. The Molecular Beam Scattering Instruments allow us to control many of these variables in order to determine the fundamental physics involve.

In this work we combine experimental measurements and theoretical calculations to understand the dynamics of Helium uptake. The calculations show that Helium will only "enter" at a specific region of the ice surface and that the absorption probability increases with the collision energy. This implies that there is an energetic barrier to Helium absorption. The experimental and trajectory absorption probability data are in qualitative agreement at high collision energies but at low collision energies the experiments show a much higher absorption probability. This may be due to the onset of an alternative adsorption mechanism at low temperature. The low temperature diffusion of Helium through amorphous solid water is consistent with an extrapolation of the diffusivities of liquid water and crystalline ice to low temperature.

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