Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First Principles Simulations of Ice Nucleation at Metal Surfaces
ANGELOS MICHAELIDES, MATTHIAS SCHEFFLER, Fritz-Haber-Institut —
Ice nucleation at solid surfaces is of relevance to countless scientific and technological processes. In particular the nucleation of ice nano-crystals on metal surfaces is often a key first step in cloud formation and corrosion [1]. Yet unfortunately this remains one of the most poorly understood natural phenomena; severely lacking in atomic level understanding. Here, we discuss detailed density functional theory studies aimed at putting our understanding of ice nucleation at metals on a much firmer footing. Specifically the properties of H_2O hexamers - the smallest 'building blocks' of ice - adsorbed on a number of close-packed transition metal surfaces have been examined. We find that the competing influences of substrate reactivity and hexamer-substrate epitaxial mismatch conspire to yield a rich variety of (novel) hexameric ice structures, some of which have been observed by recent scanning tunnelling microscopy experiments [2]. [1] H.R. Pruppacher and J.D. Klett, *Microphysics of Clouds and Precipitation*, (Kluwer, Dordrecht, 2003). [2] K. Morgenstern, *et al.*, (To be published).

Angelos Michaelides
Fritz-Haber-Institut

Date submitted: 28 Nov 2004 Electronic form version 1.4