

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

K⁺-hydration in a low-energy two-dimensional wetting layer on the basal surface of muscovite PETER J. FEIBELMAN, Sandia Natl Labs — Density Functional Theory points to a key role of K⁺ solvation in the low-energy two-dimensional arrangement of water molecules on the basal surface of muscovite. At a coverage of 9 water molecules per 2 surface potassium ions, there is room to accommodate the ions into wetting layers wherein half of them are hydrated by 3 and the other half by 4 water molecules, with no broken H-bonds, or wherein all are hydrated by 4. Relative to the “fully connected network of H-bonded water molecules” that M. Odelius *et al.* [Phys. Rev. Lett. **78**, 2855– 2858 (1997)] found to form “a cage around the potassium ions,” the hydrating arrangements are several tens of meV/H₂O better bound. Thus, low-temperature wetting on muscovite is not driven towards “ice-like” hexagonal coordination. Instead, solvation forces dominate.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Peter Feibelman
Sandia Natl Labs

Date submitted: 06 Nov 2013

Electronic form version 1.4