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/H\(_2\)O better bound. Thus, low-temperature wetting on muscovite is not driven towards “ice-like” hexagonal coordination. Instead, solvation forces dominate.

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