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Tuning the diamond surface from hydrophobic to superhydrophilic by submonolayer surface modification[1] SHENG MENG, Physics, University of Texas at Austin and Physics, Harvard University, ZHENYU ZHANG, Condensed Matter Sciences Division, Oak Ridge National Lab, EFTHIMIOS KAXIRAS, Physics, Harvard University — The extreme limits of wettability, superhydrophilic and superhydrophobic behavior, are useful in industrial applications such as anti-fogging and self-cleaning. Superhydrophilic behavior is highly desirable in biomedical applications, protecting biomolecules from damage in their interaction with biomaterials. While substantial progress has been made in designing superhydrophobic materials, relatively little effort has been devoted to the development of superhydrophilic materials, particularly biocompatible ones. Here we show, using first-principles calculations, that the water affinity of an initially highly hydrophobic H-passivated diamond (111) surface can be drastically altered with introducing a fraction of a monolayer of alkali metals. In particular, terminating the diamond surface with F and replacing 1/3ML F by Na, or introducing one third monolayer of Li and methylating half of the remaining surface sites, produces stable surfaces with superhydrophilic behavior which are perfect candidates for biomedical applications.

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