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First-Principles Investigation on Water dynamics at Functionalized Silicon surface[1] DONGHWA LEE, ERIC SCHWEGLER, Lawrence Livermore Natl Lab, YOSUKE KANAI, The University of North Carolina at Chapel Hill — Interfacial water behavior at semiconductor surfaces is one of the most important areas of investigation for diverse industrial applications such as crystal growth, lubrication, catalysis, electrochemistry and sensors. Although the hydrophobicity at surface is widely recognized to be important in determining the behavior of water molecules near the surface, we show that subtle molecular details may also play a role in determining the dynamical behavior of water by employing first principles molecular dynamics simulations. By comparing water diffusivity at three non-polar surfaces, we find that water diffusivity is significantly faster near the H-terminated surface as compared to either CH3- or CF3-terminated surfaces. By examining the interfaces in detail, we find that the specific surface corrugation that is characteristic of the H-terminated surface leads to a suppression of hydrogen bond network ring structures by enhancing hexagonal spatial distribution of water molecules near the surface. Such a distinct molecular dependent behavior of the interfacial water was found to persist well into the liquid, while the most structural properties are noticeably influenced in only the first water layer (∼5 Å).

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Donghwa Lee
Lawrence Livermore Natl Lab

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