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Quantum Monte Carlo calculations of the energy-level alignment at organic-inorganic hybrid interfaces[1] ZHIGANG WU, YOSUKE KANAI, JEFFREY GROSSMAN, University of California at Berkeley — Understanding interface properties of nano- and hybrid- materials at molecular level is of critical importance for fostering technological advancements. While the density functional theory (DFT) continues to be an important method for investigating opto-electronic and excitation properties of materials, the DFT calculations in some cases fail to provide an accurate description. One such difficult case is computing the energy-level alignment at a hybrid interface, composed of two distinct materials with very different electronic characteristics. In this work we present a quantum Monte Carlo approach to correct the Kohn-Sham (KS) level alignment, and we demonstrate this approach for hybrid interfaces between the silicon (001) surface and several organic molecules. Our calculations show that for some molecules there is a qualitative difference with the DFT-KS level alignment, completely changing the character of the heterojunctions formed. We will discuss its implication for understanding the opto-electronic behaviors of hybrid interfaces, along with some computational/theoretical challenges in extending this approach further.

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