Structural, electronic, and non-equilibrium charge transport properties of silicon-polymer interfaces

JOSEPH TURNBULL, North Carolina State University, Department of Physics, Center for High Performance Simulation, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Department of Physics, Center for High Performance Simulation; Oak Ridge National Laboratory — There is great interest in developing silicon-based electronic devices incorporating organic molecules as active components. In order to glean insights for applications of such devices in molecular electronics and photovoltaics contexts, we study paradigmatic organic-inorganic interfaces using first-principles calculations for pi-conjugated polymers in contact with H-passivated silicon surfaces. We describe the morphological and electronic properties of these hybrid structures, including interfacial charge transfer, band alignment, and non-equilibrium charge transport.

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