

Abstract Submitted  
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**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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