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Electronic Coupling of Organics to Semiconductors Through Quantum Resonance GUILLUAME DUPONT, CHARLES MUSGRAVE, Stanford University — We have simulated attaching various organic species to semiconductor surfaces for the formation of molecular electronics and sensors using DFT. Although strong attachment and limited decomposition of the molecular species to Si and Ge surfaces is often achieved, the electronic structure of the molecular-semiconductor interface is not suitable for many devices. We have found that certain organics are stabilized on semiconductor surfaces by quantum mechanical resonance. In some cases, this enhances the growth of organic nanowires and other structures. Furthermore, this resonance leads to stronger electronic coupling between the attached organic and the semiconductor substrate which might be useful in improving electrode-molecule charge injection for molecular transistors and sensors. We will present several examples to illustrate the effect as well as to provide general guidelines for determining how to design molecules to exhibit this property for attachment to Si and Ge.

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