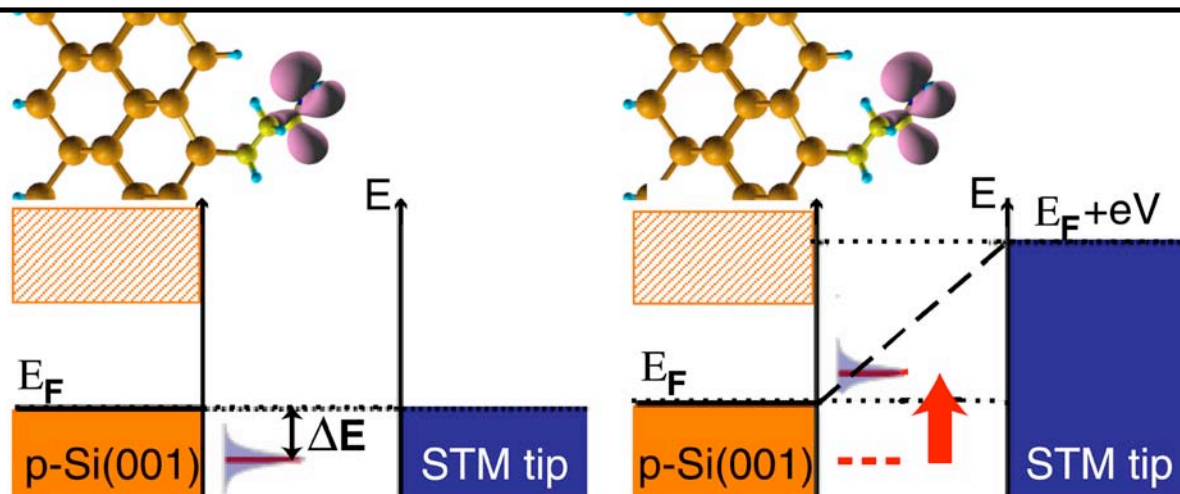


Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Assessing negative differential resistance in organic-silicon systems



Negative differential resistance (NDR) has been proposed to arise in silicon-based molecular systems through field-induced movement of a frontier molecular level into the Si band gap. We used a first principles approach to assess quantitatively the viability of this mechanism in organic-Si systems. In particular, NDR was recently reported in cyclopentene on p-type Si(001) using low temperature scanning tunneling microscopy experiments. As variance with the proposed mechanism, our calculations indicate that the frontier energy levels are independent of applied electric fields. Our work rules out a field-induced movement of frontier levels as the mechanism for NDR, at least in this case. However, we find that such a mechanism may occur for systems involving simple modifications of cyclopentene that incorporate lone pairs. One such system is amino-cyclopentene on Si(001) (shown above). Our results should provide guidelines for the design of molecules exhibiting NDR.