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Geometric Effects on the Tunneling Apparent Barrier Height
ARAN GARCIA-LEKUE, THOMAS FREDERIKSEN, DIPC, Donostia International Physics Center, ANDRES ARNAU, Centro de FIsica de Materiales — An experimental quantity which may help understanding the mechanism of electron tunneling, in STM experiments or across broken nanojunctions for example, is the apparent barrier height. In order to extract information from this experimental observable one can consider a simple one-dimensional tunneling model, where the apparent barrier height is the rate of change of the logarithm of the conductance with the tip-apex separation or vacuum gap. Theoretically, a faithful analysis of the apparent barrier height requires a precise description of the tunneling conductance in the vacuum region. However, most of the conductance calculations are performed using atom centered localized basis sets, which cannot adequately describe the tunneling current crossing the vacuum gap and can therefore lead to erroneous results. In this work, we present tunneling conductance calculations obtained using the transport calculation method introduced in Ref. [1]. Since this method employs a plane-wave basis set, it provides accurate results for the electron tunneling across the vacuum gap and, consequently, for the apparent barrier height. Here, we report results for broken Au nanojunctions with different geometries, which allows us to thoroughly investigate geometric effects on the apparent barrier height. 1. A. Garcia-Lekue and L.W. Wang, Phys. Rev. B. **74**, 245404 (2006).

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