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Plane-wave based Electron Tunneling through Au nanojunctions
ARAN GARCIA-LEKUE, DIPC (Donostia International Physics Center), LIN-WANG WANG, LBNL (Lawrence Berkeley National Laboratory) — A faithful theoretical analysis of the electron tunneling across nanojunctions 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 wave function in the vacuum region and can therefore lead to erroneous results. In this work, we present tunneling conductance calculations obtained using the transport calculation method introduced in Refs. [1,2]. Since this method employs a plane-wave basis set, it provides accurate description for the electron wave functions in all real space. We will report results for broken Au nanojunctions with different geometries, which allows us to thoroughly investigate geometric effects on the apparent barrier height. Such quantity, which is closely related to the electron tunneling mechanism, is experimentally accessible by STM experiments or across broken nanojunctions.

[1] L.W. Wang, Phys. Rev. B **72**, 045417 (2005).
[2] A. Garcia-Lekue and L.W. Wang, Phys. Rev. B **74**, 245404 (2006).

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