

Abstract Submitted  
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**Single channel conductance of  $H_2$  molecules** VICTOR MANUEL GARCIA-SUAREZ, Lancaster University, ALEXANDRE REILY ROCHA, Trinity College Dublin, STEVE BAILEY, COLIN LAMBERT, Lancaster University, STEFANO SANVITO, Trinity College Dublin, JAIME FERRER, Universidad de Oviedo, UNIVERSIDAD DE OVIEDO COLLABORATION, TRINITY COLLEGE DUBLIN COLLABORATION, LANCASTER UNIVERSITY COLLABORATION — We report a detailed theoretical study of the atomic arrangement and conduction channels of an  $H_2$  molecule joining either Platinum or Palladium electrodes. We find that the bonding state of the molecule does not hybridize with the leads if the molecule forms a bridge, thereby providing a single conductance channel. On the contrary, both channels hybridize heavily, leading to high conductances, if the molecule lies perpendicular to the electrodes,. We propose that the occurrence of additional transitory peaks in conductance histograms of Pd electrodes are due to the dissolution of Hydrogen atoms in the neighborhood of the bridge, which form metastable states.

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