Mechanically-induced spin-polarization in non-magnetic metal nanocontacts

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Symmetry breaking can lead to exotic and potentially technologically useful phenomena, even in materials that are non-magnetic. For example, the Shockley surface state manifests on an exposed surface of Au111 as a result of Rashba spin-orbit (SO) splitting [1]. Other recent examples are the non-trivial edge and surface states that manifest in strong-SO topological insulators [2]. More recently, and also of great interest, is the socalled chirality-induced spin selectivity (CISS) effect in molecular nanojunctions containing chiral organic molecules [3]. The CISS effect has been attributed to symmetry breaking at the metal-molecule interface [4]. In this work, using a Gaussian-type orbital (GTO) density functional theory (DFT) approach [5] to obtain SO-corrected bands (see Fig 1), allowing the efficient modelling of complex nano-structures which are intractable by other methods, we show that strong spin-polarization can manifest even in non-magnetic metal nanocontacts where centro-symmetry is broken by simple mechanical rotation (see Fig. 2). Our results are likely to form the basis for insights into more complex systems, such as the molecular nanojunctions in which the CISS effect is important.

References

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Figures

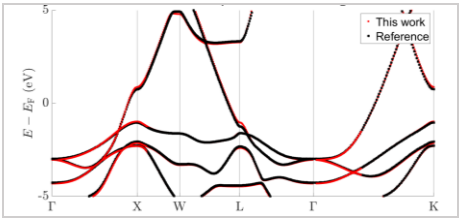

Figure 1: Comparison of SO-corrected bands about the Fermi level obtained using our method (red) and a reference method (black) for face-centred cubic Au.

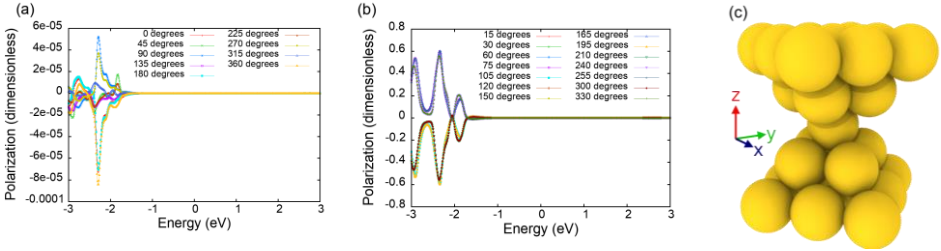

Figure 2: Spin-polarization at (a) highly symmetric and (b) unsymmetric angles as one end of a simple Au9-Au4-Au-Au4-Au9 nanocontact (c) is rotated about the *z*-axis. In (c), the top half has been rotated by 45° with respect to the bottom.