

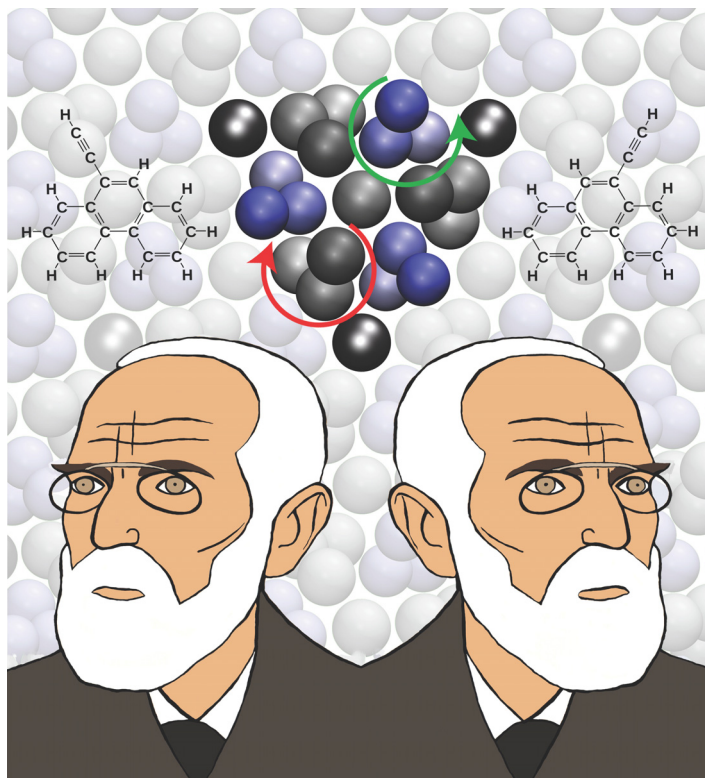
Role of van der Waals interactions in the enantioselectivity of PdGa(111) surfaces

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We investigate, by means of first-principles calculations, the origin of the enantioselectivity of the PdGa(111) surface that was recently proved in the literature, for the adsorption of the small organic molecule 9-ethynylphenanthrene, through the experiments conducted by Prinz and co-workers[1]. The key ingredient to understand the experimental evidence is the appropriate description of van der Waals interactions beyond the widely employed atomic pairwise approximation[2]. A recently developed van der Waals-inclusive density-functional method[3,4], which encompasses dielectric screening effects, reveals the origin of the experimentally observed enantioselectivity and provides conclusive evidence of chiral recognition on a bimetallic surface driven by dispersion interactions. The incorporation of dielectric screening leads to a renormalization of the dispersion interaction range allowing for the appropriate weighting of the molecule-substrate interactions at intermediate distances between 2.5Å and 5Å.

References:

- [1] J. Prinz *et al. Angew. Chem.* **54**, 3902 (2015)
- [2] A. Yakutovich *et al. J. Am. Chem. Soc.*, **140**, 1401 (2018)
- [3] A. Tkatchenko, M. Scheffler, *Phys. Rev. Lett.* **102**, 073005 (2009)
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Van der Waals driven enantioselectivity of PdGa(111) surfaces. The two portraits of Johannes Diderik van der Waals are from artist Nando Crippa.