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2D vs. 1D Structures at Stepped Si Surfaces and in Organic Molecules

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The dimensionality of a structure plays an important role in its electronic properties, as demonstrated recently by a variety of layered compounds who behave very differently as single layer. This raises the question what happens when reducing the dimensionality further to one-dimensional atomic chains - the finest conceivable nanowires. Theory predicts exotic behavior, such as the elusive Luttinger liquid. Strong correlations are established between electrons propagating along an atomic chain, since they are not able to avoid each other. One might also expect reduced dielectric screening and higher chemical activity in 1D structures due to the reduced number of neighbors. This talk focuses on two types of atomically-precise structures that bridge the gap between 2D and 1D. Both their preparation and their electronic structure are considered. Stepped surfaces can be prepared on vicinal Si with great precision (less than one kink in 10⁴ edge atoms), since the high energy cost of a broken Si-Si bond leads to stable surface reconstructions. These can be decorated with a wide variety of metal atoms, frequently leading to metallic wires on a semiconducting substrate. The transition from 2D to 1D is explored by varying the step spacing. A variety of interesting phases have been found in these wires, such as charge density waves [1], spin-polarized energy bands, and an ordered array of spinpolarized Si edge atoms [2]. The other approach uses organic molecules to compare π -bonded carbon sheets and chains [3]. First-principles calculations show that 1D wires exhibit very simple molecular orbitals which mimic the overtones of a vibrating string, while 2D structures form more complex orbital patterns related to the modes of a drum. The dielectric screening is found to scale with the number of atoms in a molecule rather than the number of neighbor atoms, suggesting delocalized screening. Looking into the future, we discuss molecular complexes combining 2D and 1D structures with atomic precision, such as the donor- π -acceptor complexes used in dye-sensitized solar cells [4]. Computational screening of the energy levels for thousands of dye molecules provides the blueprint for tandem solar cells where two π -absorbers are connected by molecular wires [5].

[1] Paul C. Snijders and Hanno H. Weitering, *Rev. Mod. Phys.* 82, 307 (2010) [2] Steven C. Erwin and F. J. Himpsel, *Nature Communications* 1:58 (2010). [3] J. M. Garcia-Lastra et al., *J. Phys. Chem. C* 120, 12362 (2016). [4] A. Yella et al., *Science* 334, 629 (2011); Ioannis Zegkinoglou et al., *J. Phys. Chem. C* 117, 13357 (2013). [5] Kristian B. Ørnsø et al., *Chemical Science* 6, 3018 (2015).