

Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles - DTU Orbit (09/11/2017)

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Chemists generally believe that covalent and ionic bonds form much stronger links between atoms than the van der Waals force does. However, this is not always so. We present cases in which van der Waals dispersive forces introduce new competitive bonding possibilities rather than just modulating traditional bonding scenarios. Although the new possibilities could arise from any soft–soft chemical interaction, we focus on bonding between gold atoms and alkyl or arylsulfur ligands, RS. Consideration of all the interactions at play in sulfur-protected gold surfaces and gold nanoparticles is necessary to understand their structural, chemical and spectroscopic properties. In turn, such knowledge opens pathways to new chemical entities and innovative nanotechnological devices. Such experimentation is complemented by modern theory, and presented here is a broad overview of computational methods appropriate to fields ranging from gas-phase chemistry to device physics and biochemistry.

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