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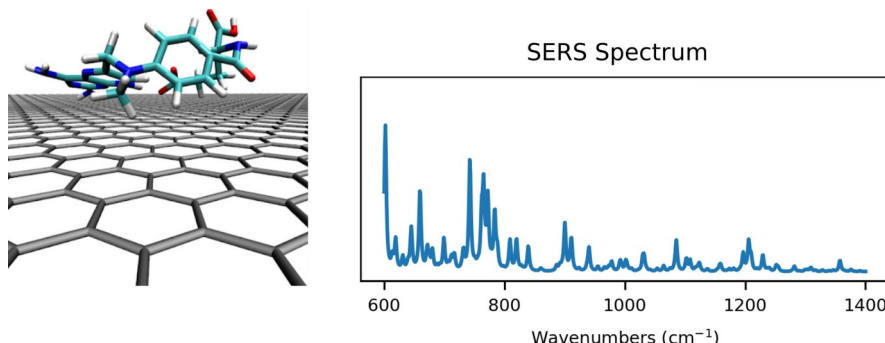
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# Surface-Enhanced Raman Scattering: Insights from Atomistic Modelling

The optical response of plasmonic nanostructures can be tuned by varying their shape, size, and chemical composition [1]. Peculiar phenomena arise when a molecular system is adsorbed on the surface of plasmonic materials, ranging from surface-enhanced spectroscopies to photocatalysis [2]. The accurate description of the optical properties of the plasmonic substrates is thus crucial for an understanding of the physical phenomena occurring at the plasmon resonance frequency.

Here, we present a fully atomistic, yet classical, approach to predict the plasmon properties of nanostructures of complex shapes. The method is general enough to describe any plasmonic material, including noble metal nanoparticles (Ag and Au) [3] and metal alloys [4]. We show that our classical approach for plasmonics can correctly reproduce reference *ab initio* data [3,5], and experimental trends [3-4], and can be applied to large-scale nanoplasmonic simulations [6]. The method is also coupled to a quantum mechanical (QM) description of the molecular system adsorbed on the nanostructure surface [5]. The resulting mixed QM/classical method is then extended to various spectral signals, from surface-enhanced Raman scattering [7-8] to surface-enhanced fluorescence [8].



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