Machine learning for molecular design of plasmonic nanosystems

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The interaction between molecules and strongly confined electromagnetic fields at metallic nanostructures results in extreme enhancement of molecular spectroscopic signals. This effect can be utilized in new nanoscale devices such as molecular terahertz (THz) detectors. However, to achieve high efficiency, molecules with highly specialized properties are required. We explore how quantum chemistry and machine learning methods can provide good candidate molecules for these applications. In particular, we investigate a promising new THz detection technique based on frequency upconversion by molecular vibrations, as demonstrated in Ref. [1]. By screening databases containing millions of molecules, a two-orders-of-magnitude improvement of spectral intensity can be achieved [2]. We introduce an interactive online tool, Molecular Vibration Explorer [3], that enables further analysis of our quantum chemistry results for a wide range of surface-enhanced spectroscopic applications. Generative machine learning provides a route for going beyond existing molecular databases, to instead design new functional molecules by biasing towards the desired properties [4]. We discuss how recent developments in conditional generative design [5] open the way for the targeted generation of functional molecules.

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