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Poster: Computationally efficient methods for studying strong coupling in cavities

Strong coupling between molecules and electromagnetic cavities is commonly studied using few-level quantum models, such as the Jaynes–Cummings or Dicke models, which describe matter in a highly simplified way. Alternatively, there are first-principles approaches such as time-dependent density-functional theory (TDDFT) and quantum-electrodynamical density-functional theory (QEDFT), which are computationally very costly. Here, we explore methods that have low or intermediate computational cost, yet still retain material specificity. Using only dipolarly coulpled polarizable units in a classic electrostatics framework, we are able to almost quantitatively reproduce optical spectra of strongly coupled nanoparticle-molecule assemblies [1]. Training neuroevolution potentials (NEPs) for predicting the energetic landscape, as well as permanent dipoles of molecules, we are able to study the modification of chemical reaction rates in cavities [2].

References:

[1] J. Fojt, T. P. Rossi, T. J. Antosiewicz, M. Kuisma, P. Erhart, J. Chem. Phys. (2021).
[2] C. Schäfer, J. Fojt, E. Lindgren, P. Erhart, to be submitted (2023).

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