Intermolecular Pair Potentials in Cavity Quantum Electrodynamics

John P. Philbin[1] and Prineha Narang[1]

[1] *Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, United States*

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The prospect of controlling chemical processes via strong light-matter coupling has recently been the subject of much theoretical and experimental interest. In this work, we utilize perturbation theory, *ab initio* cavity quantum electrodynamics coupled cluster calculations, and neural networks to develop the first intermolecular pair potentials for molecules inside of optical cavities that can be used to study the structural and thermodynamic properties of molecules in condensed phases. Our perturbation theory analysis shows that homonuclear diatomic molecules (e.g. H_2 molecules) have new intermolecular interactions that scale with the distance between the molecules (R) as R^{-3} and R^0 inside optical cavities in addition to the typical attractive R^{-6} and repulsive short range interactions compromising a standard Lennard-Jones potential. Our intermolecular pair potentials that take into account these new interactions can be readily used in molecular dynamics simulations to understand how strong light-matter coupling inside cavities impacts chemical phenomena in condensed phases such as solid-to-liquid phase transitions.