Can we control chemistry with a cavity? Insights from molecular dynamics computer simulations

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For over a decade, experiments on molecules in Fabry-Pérot cavities have suggested changes to their reactivity in ground and excited states.[1] While these changes have been attributed to hybridization of the confined light modes of the cavity and the excitations of the molecules into polaritons due to strong light-matter coupling, there is no consensus on why such hybridization would change the chemistry. To help finding such concensus, we have combined the traditional Tavis Cummings model[2] with our own hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) non-adiabatic molecular dynamics (MD) methodology for excited-state dynamics in proteins.[3] After presenting our model,[4] we will share results that demonstrate how strong coupling affects ultra-fast excited-state proton transfer,[5,6] We will conclude the talk with an idea on how polaritons could be leveraged for mimicing biological light-harvesting.

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References

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