

Operational impact of quantum resources in chemical dynamics

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Quantum coherence and other non-classical features are widely discussed in chemical dynamics, yet it remains difficult to quantify when such resources are operationally relevant for a given process and observable. While quantum resource theories provide a principled way to compare “resource-free” and “resourceful” descriptions, most existing tools focus on state-based measures or constraints under restricted operations, rather than on the maximal influence a chosen resource can exert under fixed open-system dynamics. Here we introduce task-specific, process level quantifiers that provide computable upper bounds on the largest change a quantum resource can induce in a target figure of merit. The central idea is to compare the same dynamics acting on an initial state and on a paired, resource-free baseline that represents the closest “classical” counterpart for the task at hand. This yields a direct benchmark for the operational relevance of the resource for the chosen observable. We illustrate the framework on representative models including excitation energy transfer and derive theoretical bounds that identify conditions under which initial delocalization can, or cannot, improve trapping performance relative to incoherent preparations. Overall, the approach provides a general toolbox for diagnosing and benchmarking quantum-resource effects in chemical processes.

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