

EuCompChem2025 – Samuele-Botticelli – Oral

We introduce a new extension of the Mapping Approach to Surface Hopping (MASH) method, called Semifocused MASH (SMASH). To assess its accuracy, we compare SMASH with the Fewest Switches Surface Hopping (FSSH) method, both with and without decoherence corrections, on various molecular systems. Our results show that SMASH reproduces population dynamics with similar accuracy, while significantly reducing unphysical transitions involving large energy gaps. These findings establish SMASH as a viable approach for simulating nonadiabatic molecular dynamics.

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