

Supplementary Materials: The UV-Visible Absorption Spectra of Coumarin and Nile Red in Aqueous Solution: A polarizable QM/MM study

Tommaso Giovannini,^{*,†} Matteo Ambrosetti,[‡] and Chiara Cappelli[‡]

*†Department of Physics, University of Rome Tor Vergata, and INFN, Via della Ricerca
Scientifica 1, 00133, Rome, Italy*

‡Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy.

E-mail: tommaso.giovannini@uniroma2.it

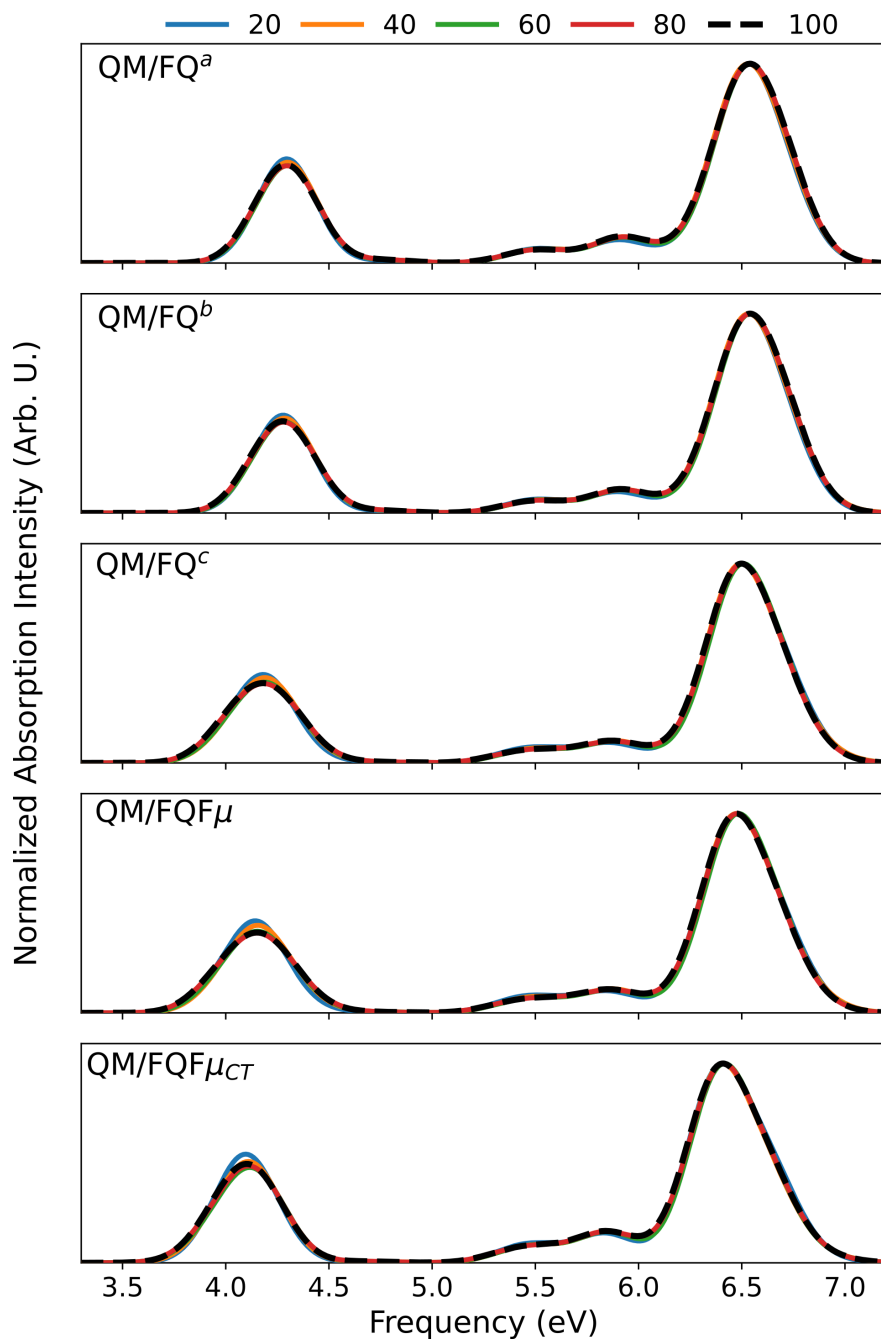


Figure S1: 7-methoxycoumarin QM/FQ^a, QM/FQ^b, QM/FQ^c, QM/FQF μ , and QM/FQF μ_{CT} UV-Vis spectra as a function of the number of snapshots, from 20 to 100.

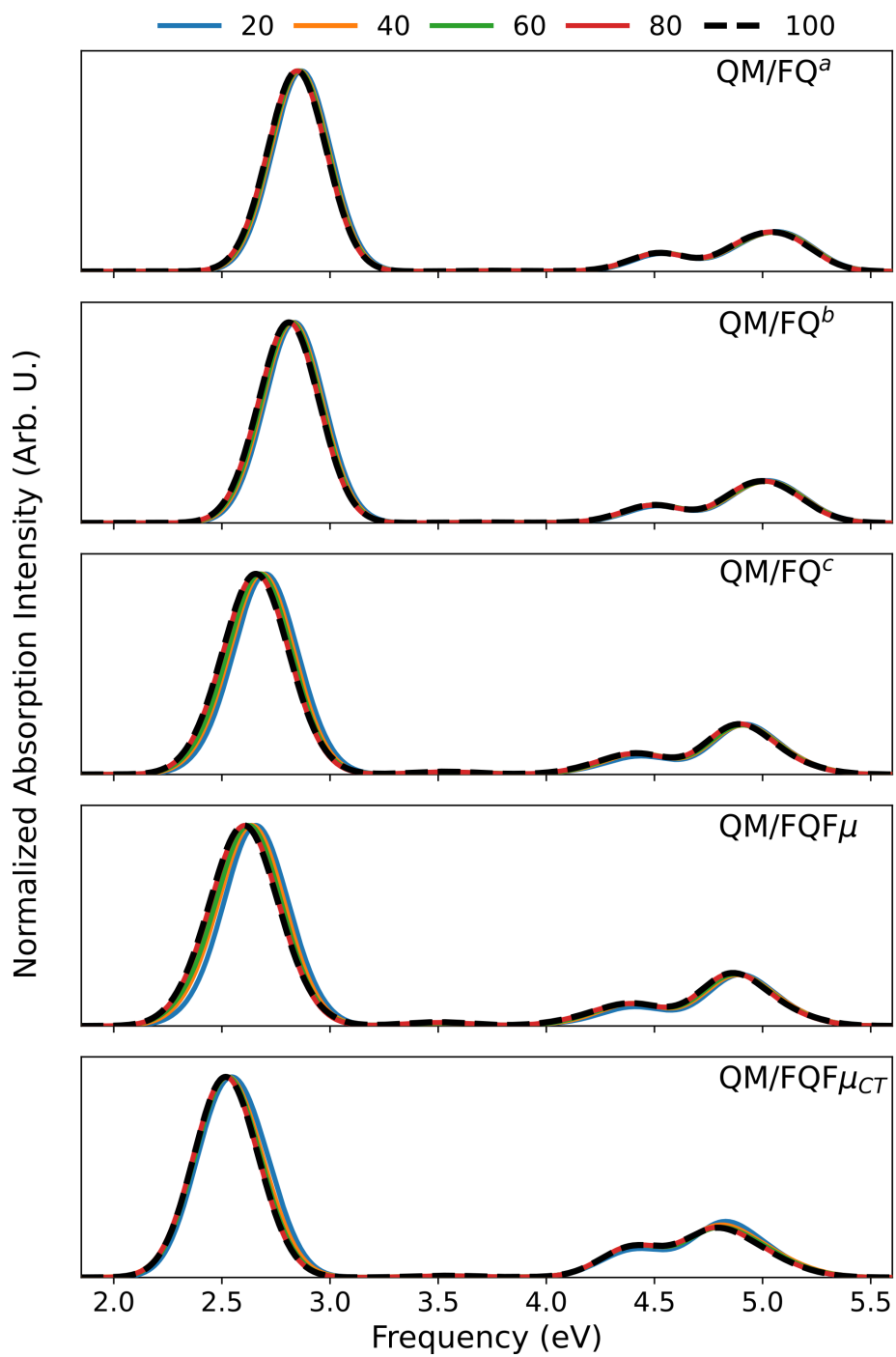


Figure S2: Nile red QM/FQ^a, QM/FQ^b, QM/FQ^c, QM/FQF μ , and QM/FQF μ_{CT} UV-Vis spectra as a function of the number of snapshots, from 20 to 100.

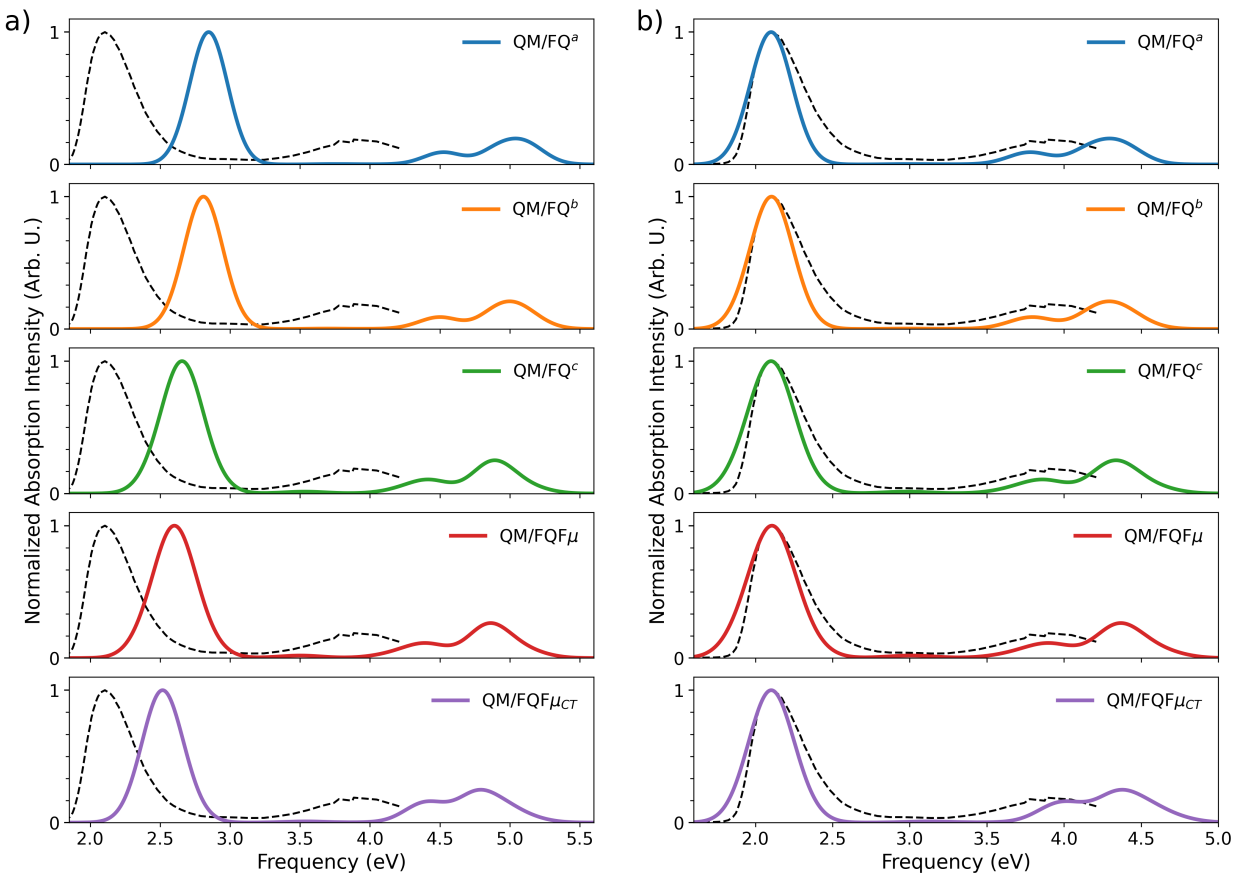


Figure S3: (a-b) Nile red QM/FQ^a , QM/FQ^b , QM/FQ^c , $QM/FQF\mu$, and $QM/FQF\mu_{CT}$ computed UV-Vis spectra. The experimental spectrum from Ref. ? is also depicted as a black dashed line. In (b) panel, the computed spectra are shifted to match the experimental main peak.