General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra

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Streszczenie

An effective time-independent approach to compute vibrationally resolved optical spectra from first principles is generalized toward the computation of one-photon electronic spectra induced by either electric or magnetic transition dipoles or by their mutual interaction. These encompass absorption, emission, and circular dichroism spectra. Additionally, the proposed computational scheme is extended to cover a broad range of approximations to evaluate vibronic transitions within both vertical and adiabatic frameworks and to be able to take into account the effects of the temperature. The presented computational tool is integrated into a general purpose computational chemistry package and offers a simple and an easy-to-use way to evaluate one-photon electronic spectra, starting from electronic structure calculations chosen according to the system under study, from fully quantum mechanical descriptions to discrete/continuum quantum mechanical/MM/polarizable continuum models.

Adres publiczny

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https://www.acs.org/content/acs/en.html