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The broadening effects on para-Nitroaniline' two-photon absorption cross-section. TARCIUS RAMOS, Instituto de Fisica, Universidade de Sao Paulo, DANIEL DA SILVA, Departamento de Ciencias da Natureza, Matematica e Educacao, Universidade Federal de Sao Carlos, SYLVIO CANUTO, Instituto de Fisica, Universidade de Sao Paulo — The theoretical two-photon absorption (TPA) cross-section depends on the incident photon energy (ω), the TPA transition probability (δ) and the spectral broadening (Γ). The ω and δ are obtained employing the quantum-chemical calculations, however it is not well defined a procedure to obtain Γ. This broadening must cover the homogeneous and inhomogeneous effects due to temperature and interactions with the environment, being the value of 0.1eV often used. We propose a way to obtain the TPA from molecular simulations, fitting the Γ to obtain equivalent theoretical and experimental spectra. The TPA of the para-Nitroaniline (pNA) was calculated for three solvents using our procedure with the rigid Monte Carlo (MC) simulation. Our theoretical values are less than 25% higher than experiment. We also performed expensive ab initio BOMD simulations of the pNA isolated and in explicit water and the results of TPA cross-section are equivalent with those obtained by MC. The broadening effects were also analysed from the variance of the transition energies using BOMD simulations and the results found again to be equivalent. The interaction effects between pNA and the water solvent increases the spectral broadening by 0.15eV compared with the isolated case.

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