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Nonlinear optical response of multiply ionized noble-gas atoms
MARYAM TARAZKAR(1,3), DMITRI ROMANOV(2,3), ROBERT LEVIS(1,3), (1) Department of Chemistry, (2) Department of Physics, and (3) Center for Advanced Photonics Research, Temple University — Calculation of dynamic polarizabilities and hyperpolarizabilities of ionized species using *ab initio* methods presents computational and conceptual difficulties, as these ionized species often have open-shell electronic system. We use multi-configurational self-consistent field (MCSCF) method with extended basis sets for calculating dynamic polarizability and second-order hyperpolarizabilities of atomic noble gases and their multiply charged cations in non-resonant regime. The calculations were performed at wavelengths ranging from about 100 nm to the red of the first multi-photon resonance all the way toward the static regime. The results were benchmarked to those of CCSD calculations for ions of even-number charge. The second-order hyperpolarizability coefficients were found to decrease when the electrons are progressively removed from the system. At higher ionization states, these coefficients become less dispersive as a function of wavelength. The values and even the signs of the $\gamma^{(2)}$ coefficients were found to depend on the spin of the ionic quantum state. Thus, for Ne^{+3} and Ne^{+4}, in low-spin states (^2P_u, and ^1S_g, respectively) the sign of $\gamma^{(2)}$is positive, whereas in high-spin states (^4S_u, and ^3P_g) the sign is negative. The calculated hyperpolarizabilities of multiply ionized atoms relate to experiments on very bright high-order harmonic generation in multiply ionized plasmas (D. Popmintchev *et al.*, *Science*, **350** (6265), 1225 (2015)).

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