State-of-the-art ab initio studies of photoassociation schemes for production of cold calcium molecules

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State-of-the-art *ab initio* techniques have been applied to compute all potential energy curves for the excited states of the calcium dimer in the Born-Oppenheimer approximation corresponding to four lowest atomic dissociations, ^{3}P + ^{1}S, ^{3}D + ^{1}S, ^{1}D + ^{1}S, and ^{1}P + ^{1}S. The potential energy curves were computed using a combination of the equation-of-motion approach within the coupled-cluster singles and doubles framework for the valence-core electronic correlation and of the full configuration interaction for the valence-valence correlation. The potentials were corrected for the relativistic terms resulting from the many-electron Breit theory to the first-order in α^2. The spin-orbit coupling matrix elements with the full spin-orbit Hamiltonian and the nonadiabatic coupling terms were obtained from the complete active space selfconsistent field calculations. The electric transition dipole moments governing the transitions to the ground $X^1\Sigma_g^+$(^{1}S + ^{1}S) were computed as the first residue of the frequency-dependent polarization propagator computed with the coupled-cluster method restricted to single and double excitations. The computed points have been analytically fitted and used in nearly exact nonadiabatic calculations of the ro-vibrational energy levels and photoassociation intensities at ultralow temperatures. Our theoretical results will serve as predictions of the possible schemes for production of cold calcium molecules, as well as to interpret the measurements of the photoassociation spectra of colliding ultracold atoms and the conventional high-resolution spectra of the calcium dimer.