

BODY-FRAME COHERENCES AND ROTATIONAL-ELECTRONIC WAVE-PACKET DYNAMICS OF CAF IN NON-PENETRATING RYDBERG STATES

SERHAN N. ALTUNATA, and ROBERT W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA 02139.*

The time dependent wave-packet dynamics of a non-penetrating Rydberg electron in a body-frame coherent superposition state of CaF is investigated using an effective Hamiltonian model. Our results indicate that the information about the ion-core quadrupole moment can be directly inferred by monitoring the time required for the Rydberg wave-packet to return to its initial state. The effective Hamiltonian model is then embedded in a time-dependent multichannel quantum defect theory model which has the advantage of capturing all molecular resonances(i.e. the short range electron-nuclear scattering processes which lead to rotational transitions of the core) in a single, unified calculation. Both theories can be applied to quantitatively describe the data that will be provided from the ongoing time-domain experiments. Extensions to include vibrational interactions, predicted by the R-dependence of the quantum defect matrix elements, are possible and constitute the natural future directions in this work.