DISSOCIATION DYNAMICS OF THE DIAMONDOID ADAMANTANE UPON PHOTOIONIZATION BY XUV FEMTOSECOND PULSES

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Abstract. This work presents photodissociation studies of the diamondoid adamantane using extreme ultraviolet (XUV) femtosecond pulses. Lately, diamondoids are attracting increasing interest for use as an applied nanomaterial (Stauss *et al.*). Further, diamondoids have been found to be the most abundant component of presolar grains in space, and due to their high stability they are thus also expected to be abundant in the interstellar medium (Anders *et al.*, Henning *et al.*).

I will present a recent study (Maclot *et al.*), in which we demonstrate that the dissociation dynamics of adamantane dications takes place in a two-step process: barrierless cage opening followed by Coulomb repulsion-driven fragmentation. The experiment was carried out at the Intense XUV beamline at the Lund Laser Centre, where high-flux high-order harmonics are generated with photon energies up to 60 eV, pulse energies in the J regime and pulse durations on the femto- and attosecond time scale (Manschwetus *et al.*). To get insight into the dynamics, we use a theoretical approach combining potential energy surface determination, statistical fragmentation methods and molecular dynamics simulations. We found that the most stable structures of the dication exhibit an open-cage geometry at ∼4 eV below the double ionization threshold, that can be reached in a few tens of femtoseconds after the ionization. However, these structures are metastable and dissociate into several fragments in a Coulomb repulsion process.

References

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