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Coulomb explosion of alkali dimers on a superfluid 4HeN droplet: a 4He-TDDFT simulation

We simulate the Coulomb explosion upon double ionisation of alkali dimers (Ak2, Ak≡ Na, Rb, Cs) bound to the surface of a superfluid droplet of 1000 to 50000 4He atoms, using 4He-TDDFT (Francesco et al. [1]) This work was motivated by the experiment of Kristensen et al. [2], who used this process to deduce the abundance ratio of neutral dimers formed on the surface of a helium nanodroplet in either the singlet X 1Σ+g or the triplet a 3Σ+u electronic state. 4He-TDDFT is a semi-empirical method describing the helium density at equilibrium (static version) or during real time dynamics, which has proven to be the best compromise between accuracy and the ability to simulate superfluid helium droplets of realistic size. We first obtain the equilibrium configuration of Ak2 singlet (X 1Σ+g) or triplet (a 3Σ+u) on the droplet surface. The Coulomb explosion dynamics is then initiated by switching on the Ak+-Ak+ repulsive potential. Our results confirm the experimentalists'hypothesis that the droplet does not affect the final kinetic energy of the ions very much, therefore validating the singlet to triplet ratios obtained. In addition, the influence of several parameters which contribute to the width of the kinetic energy distribution has been examined, such as the droplet size and the Ak2 vibrational or orientational zero-point motion. Finally, our results also reveal the deviation of the ions trajectories from antilinearity, an effect which can be measured and strongly depends on the droplet size.

[1] Francesco Ancilotto et al,International Reviews in Physical Chemistry,
36:4.621, 707,2017

[2] Henrik H. Kristensen, Lorenz Kranabetter, Constant A. Shouder, Christoph Stapper, Jacqueline Arlt, Marcel Mudrich, and Henrik Stapelfeldt. "Quantum state-sensitive detection of alkali dimers on helium nanodroplets by laser-induced coulomb explosion ". Phys. Rev. Lett., 128:093201, 2022

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