

## RYDBERG STATES OF ALKALI METAL ATOMS ON SUPERFLUID HELIUM DROPLETS - THEORETICAL CONSIDERATIONS

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The bound states of electrons on the surface of superfluid helium have been a research topic for several decades. One of the first systems treated was an electron bound to an ionized helium cluster.<sup>a</sup> Here, a similar system is considered, which consists of a helium droplet with an ionized dopant inside and an orbiting electron on the outside. In our theoretical investigation we select alkali metal atoms (AK) as central ions, stimulated by recent experimental studies of Rydberg states for Na,<sup>b</sup> Rb,<sup>c</sup> and Cs<sup>d</sup> attached to superfluid helium nanodroplets. Experimental spectra, obtained by electronic excitation and subsequent ionization, showed blueshifts for low lying electronic states and redshifts for Rydberg states.

In our theoretical treatment the diatomic  $AK^+-He$  potential energy curves are first computed with *ab initio* methods. These potentials are then used to calculate the solvation energy of the ion in a helium droplet as a function of the number of atoms. Additional potential terms, derived from the obtained helium density distribution, are added to the undisturbed atomic pseudopotential in order to simulate a 'modified' potential felt by the outermost electron. This allows us to compute a new set of eigenstates and eigenenergies, which we compare to the experimentally observed energy shifts for highly excited alkali metal atoms on helium nanodroplets.

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