Alkali Trimers on He Nanodroplets:
Ab initio calculations, Shell Models and Laser Spectroscopy

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A supersonic beam of helium nanodroplets (HeN = 10^4) is doped with alkali atoms, which are unique dopants as they remain on the droplet surface. Capture of multiple alkali atoms per cluster leads to molecular formation. The droplets can dissipate released binding energy very efficiently by evaporating He atoms and provide a cold environment (T=0.4 K). Whereas the formation of strongly bound low-spin molecules tends to destroy the droplet, the weakly bound high-spin van der Waals molecules (triplet dimers, quartet trimers) survive the formation process. Experimentally we have identified, in the wavelength range 10500-17500 cm^{-1}, a variety of electronic spectra of the homo- and heteronuclear trimers K_3, Rb_3, K_2Rb, KRb_2 in their quartet states.

To help the assignment we calculate the quartet manifolds of the first few electronic excitations for all these (bare) trimers with ab initio methods and provide their PES as functions of the normal modes Q_s (breathing mode) and Q_x (symmetric bending mode). We find several regular patterns in the level structure, and rationalize them in terms of harmonic-oscillator states of the three valence electrons in a quantum-dot-like confining potential.¹

For the homonuclear trimers K_3 and Rb_3 we further compute the doublet manifolds of the first electronic excitations. A simplified description of these systems as single-electron excitations in a standard electron-droplet model provides a qualitative explanation for the electronic state structure of the low-spin alkali trimers.²