Xe AND Rb ATOMS ON HELIUM NANODROPLETS: IS THE VAN DER WAALS ATTRACTION STRONG ENOUGH TO FORM A MOLECULE?

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Chemical reactions in the cold environment of a helium nanodroplet currently attract high interest and can be spectroscopically observed with typical molecular beam techniques[a]. In order to estimate the influence of surrounding helium on the van der Waals interaction between heliophilic and heliophobic dopants that could be investigated in our lab with ESR spectroscopy[b], we apply density-functional theory to simulate a double-dotation of He-clusters with Rb and Xe atoms. Simulations of a double-doped He_N droplet with N = 500 show that the alkali metal atom stays on the surface, whereas the Xe atom sits in the middle of the droplet. The van der Waals attraction between Rb and Xe is not strong enough to compensate the separation of the heliophilic Xe and the heliophobic Rb caused by the helium droplet: a potential barrier of 23.4 K has to be overcome[c], which is to be compared with the 0.4 K internal temperature of the droplet.

[a] C. Callegari and W. E. Ernst, Helium Droplets as Nanocryostats for Molecular Spectroscopy - from the Vacuum Ultraviolet to the Microwave Regime, in: Handbook of High-Resolution Spectroscopy, eds. M. Quack and F. Merkt, John Wiley & Sons, Chichester (2011)

[b] M. Koch, C. Callegari, and W. E. Ernst, Mol. Phys. 108 (7), 1005-1011 (2010)

[c] J. Poms, A. W. Hauser, and W. E. Ernst, Phys. Chem. Chem. Phys. 14, 15158-15165 (2012)