

Dissociation and Recombination Dynamics of Chromium Molecules in Helium Nanodroplets

Markus Koch, Andreas Kautsch, and Wolfgang E. Ernst

Institute of Experimental Physics, Graz University of Technology, Graz, Austria

Email: markus.koch@tugraz.at

The photoinduced dynamics of chromium dimers and small chromium clusters isolated in helium nanodroplets have been investigated with resonant multiphoton ionization (REMPI) spectroscopy and mass sensitive ion detection [1]. Electronic excitation of ground state ($X^1\Sigma_g^+$) Cr_2 molecules to an excited state ($A^1\Sigma_u^+$) induces dissociation into a ground state (a^7S_3) and a metastable (a^5S_2) atom. We find that the ground state atom remains solvated inside the droplet, while the metastable atom migrates to the droplet surface without desorbing from the droplet. This interpretation is based on the spectral REMPI signatures of both dissociation products and supported by density functional theory simulations [2]. We also find that REMPI of the surface located a^5S_2 atom induces recombination of the two Cr atoms, which is evidenced by Cr_2^+ detection. For small Cr clusters ($\text{Cr}_{3,4}$), our results indicate that they may be composed of chromium dimers that exhibit the same dissociation and recombination behavior.

This demonstration of quantum state specific dopant locations, photoinduced transitions between solvated and surface locations, and the stable separation of two dopants open a possibility for the investigation of photoinduced chemistry in helium nanodroplets.

References

- [1] A. Kautsch, M. Koch, and W. E. Ernst, accepted by PCCP (<http://dx.doi.org/10.1039/C5CP01009H>), 2015
- [2] M. Ratschek, J. V. Pototschnig, A. W. Hauser, and W. E. Ernst, *J. Phys. Chem. A* **118**, 6622, 2014