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Size-resolved, angle-dependent photoelectron spectroscopy of neutral alkali metal-doped dimethyl ether clusters: Comparison of Li and Na

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We report the first measurements of electron binding energies and photoelectron anisotropies of size-resolved, angle-dependent photoelectron spectra of lithium-doped dimethyl ether (CH_3OCH_3) clusters. Neutral clusters were studied in the range from the bare lithium atom to an average cluster size of 63 dimethyl ether molecules with a single lithium atom. Using a combination of density functional calculations and experimental spectra we explain trends in electron binding energies and photoemission anisotropies of $Li(CH_3OCH_3)_n$ clusters. The lithium-doping results are compared to a previous study [1,2] performed in our group on sodium-doped dimethyl ether clusters and found to produce similar trends in the evolution of electron binding energies and photoemission anisotropies. We are especially interested in the structural and electronic differences that arise from replacing sodium with the smaller alkali metal, lithium. In highly symmetric clusters, the highest occupied molecular orbital can delocalize over an extended region and form a symmetric charge distribution of mainly s-character, resulting in a pronounced photoemission anisotropy [1]. For $Na(CH_3OCH_3)_n$ clusters, the hexamer ($n = 6$) was shown to produce such a highly symmetric structure and pronounced photoemission anisotropy. In the case of $Li(CH_3OCH_3)_n$ clusters, the tetramer ($n = 4$) exhibits an analogously high symmetry structure with correspondingly high photoemission anisotropy. Calculation results predict highly symmetric geometries and strong s-character for the highest occupied molecular orbitals of both $Na(CH_3OCH_3)_6$ and $Li(CH_3OCH_3)_4$.

References:
[1] Adam H. C. West, Bruce L. Yoder, David Luckhaus, Ruth Signorell, J. Phys. Chem. A 2015, 119, 12376-12382.
[2] Adam H. C. West, Bruce L. Yoder, David Luckhaus, Clara Saak, Maximilian Doppelbauer, Ruth Signorell, J. Phys. Chem .Lett. 2015, 6, 1487-1492.

Summary

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