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Structure and reactivity of negatively charged platinum and palladium clusters

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Small Pt- and Pd-clusters play an important role as active sites in heterogeneous catalysis. For this reason, we are interested in their gas phase structure. Here we show the results of a joined experimental and theoretical study. Experimentally, structural information is obtained in the group of Schooss by trapped ion electron diffraction (TIED). The resulting scattering function is compared to theoretical counterparts that were obtained by structure optimization of guess structures with density functional theory.
Here, results for three different systems are presented:
For Pt_n^--clusters with n in the range from 6 to 13, guess structures were obtained by the use of genetic algorithms with empirical potentials and based on density functional theory. The set of structures was extended by literature data. By combining theory and experiment it was possible to assign the structures observed in the experiment [1].
For Pd_n^--clusters with 55 to 147 atoms, the transition from icosahedral motifs to bulk like fcc-structures [2] is considered.
Finally, we performed quantum chemical calculation to investigate the reactivity of selected truncated octahedral Pt_n-clusters with oxygen [3].
[1] Bumüller, D.; Yohannes, A. G.; Kohaut, S.; Kondov, I.; Kappes, M. M.; Fink, K.; Schooss, D. J. Phys. Chem. A 2022, 126, 3502 doi:10.1021/acs.jpca.2c02142
[2] Kohaut, S.; Rapps, T.; Fink, K.; Schooss, D. J. Phys. Chem. A 2019, 123, 10940 doi:10.1021/acs.jpca.2c02142
[3] Yohannes, A. G.; Fink, K.; Kondov, I. Nanoscale Adv. 2022 doi:10.1039/d2na00490a

Category

Other

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