The Complex Nonmetal-to-Metal Transition in Zinc Clusters

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Divalent metal clusters are known to exhibit a nonmetal-to-metal transition as a function of size. Small clusters exhibit a pronounced band-gap, which can be well observed by photoelectron spectroscopy on cluster anions [1-3]. With increasing size this gap shrinks until it vanishes at a material dependent size, which has been interpreted as the onset of metallicity. In a combined experimental/theoretical study on zinc clusters we could now show that the situation is much more complex: for some seemingly metallic particles metallic and insulating phases exist within the same particle; furthermore most of the particles exhibit a core-shell structure with a very weak interaction between the core and the shell, which can even lead to different symmetry properties of both regions[4].

The results demonstrate that there is no welldefined and abrupt transition from an insulator to a simple metal, but rather a large transition region where the clusters exhibit properties very unusual both for insulating and metallic systems.

References

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Figure 1: Putative ground state structures of different zinc clusters and comparison of measured photoelectron spectra with calculated density of states. Blue spheres indicate weakly bound atoms; yellow spheres core regions uncoupled from the shell region (red spheres). From [4].

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