PES and DFT Study of Transition mono and bimetallic clusters

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It is clear that the determination of the geometric structure of TM clusters is a vital step towards understanding cluster properties. Therefore any effort in this direction is vital for the future possible applications and thus the development of new technologies. We present interesting results on mono and bimetallic clusters of Rh, Co, RhCo and AuRh small clusters, with regards to their electronic, magnetic and catalytic properties. These systems are interesting as doping with transition metal atoms strongly changes the properties of the host cluster. The geometric structures, relative stabilities, magnetic moments, and vibrational spectra have been systematically studied and compared to experimental Anion Photo Electron results for some cases. The results here presented have been done within the density functional theory (DFT) framework [3,4]. Our results show that H adsorption on small clusters is different than in bulk, on the other hand the transition metal doping of gold clusters plays a special roll in their stabilities and their chemical activity. And we found interesting behavior of their magnetic moment as Co is successively added to Rh clusters.

[1] W. Bouwen, F. Vanhoutte, F. Despa, S. Bouckaert, S. Neukermans, L. T. Kauhn, H. Weidele, P. Lievens, R. E. Silverans, Chem. Phys. Lett. 314, 227 (1999)
[2] M. Heinebrodt, N. Mailinowski, F. Tast, W. Branz, I. M. L. Billas, T. P. Martin, J. Chem. Phys. 110, 9915 (1999)
[3] TURBOMOLE V6.5
[4] Gaussian09