Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Not so loosely bound: temperature dependent vibrational fingerprints of Au_NKr_M clusters LUCA M. GHIRINGHELLI, PHILIPP GRUENE, GERARD MEIJER, ANDRÉ FIELICKE, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — In order to interpret the vibrational spectra of *neutral* Au_NKr_M clusters, as measured in a Multiple Photon Dissociation Far-IR experiment (P. Gruene *et al.*, Science **321**, 674 (2008)), we calculated their finite temperature vibrational spectra, by means of all electron density functional theory, including the Tkatchenko-Scheffler van der Waals correction. We surprisingly find that Kr forms weak chemical bonds (binding energy around 0.2 eV per Kr atom) with 1- to 3-fold coordinated Au atoms belonging to small Au_N clusters ($N \leq 4$). Such Au_NKr_M clusters have a vibrational spectrum which is different from the related Au_N clusters. For bigger Au_N clusters, Kr physisorbs to the clusters, forming a complex whose vibrational spectrum is practically identical to the spectrum of the bare cluster. Anharmonicities affect the spectrum by changing (with respect to the harmonic spectrum) the relative intensity of the peaks and by showing new peaks, due to interactions among eigenmodes.

Luca M. Ghiringhelli
Fritz Haber Institute of the Max Planck Society,
Faradayweg 4-6, 14195 Berlin, Germany

Date submitted: 01 Dec 2009 Electronic form version 1.4