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Metal ad-cluster morphology vs. size on graphene/Ir(111)[1] PETER J. FEIBELMAN, Sandia National Laboratories — The chemical activity of Au clusters adsorbed on oxides depends on how many Au atoms constitute a cluster, and on the clusters' morphology and charge [1]. This makes it interesting to study the systematics of the d-band metal clusters recently discovered to grow in regular arrays on a graphene/Ir(111) template [2]. Local density functional optimization of Ir clusters on this template accurately accounts for the observed transition from 2- to 3-dimensional at a cluster size of N=26 atoms [3]. New calculations for Au clusters imply that the transition to a 3-dimensional morphology occurs for smaller N. Wetting is the issue; it is governed by the relative strength of the ad-metal bonds with itself, as against its bonds with a buckled graphene sheet. [1] H. Häkkinen, S. Abbet, A. Sanchez, U. Heiz, and U. Landman, Angew. Chem. Int. Ed. 42, 1297(2003). [2] A. T. N'Diaye, T. Gerber, C. Busse, J. Mysilvecek, J. Coraux, T. Michely, New J. of Phys. 11, 103045(2009). [3] P. J. Feibelman, Phys. Rev. B80, 085412(2009).

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