

Abstract Submitted
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Magnetism in Gold Nano-clusters¹ R.J. MAGYAR, V. MUJICA, INEST Group, Philip Morris USA Postgraduate Research Program and NIST, C. GONZALEZ, NIST, M. MARQUEZ, Philip Morris USA Research Center — Intrinsic magnetism in thiolated and unthiolated gold nano-clusters is explored from a first-principles perspective. The computed electronic structures elucidate the relevant mechanism whereby these nano-clusters develop a permanent magnetic moment. Polarized ground states are favorable due to surface paramagnetism, and bare clusters are expected to be magnetic for Au₃₈ and larger. How the thiolates effect the magnetic moment is also considered.

¹This research has been conducted by the INEST (Interdisciplinary Network of Emerging Science) group, Philip Morris USA Postgraduate Research Program

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