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A Density Functional Method for the Calculation of the Zero-Voltage Conductance of Molecular Electronic Devices

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Molecular electronics poses a new challenge to density functional theory. The key property of molecular electronic devices is their conductance g. Here we propose a new strategy for the calculation of g, employing Kohn-Sham density functional theory. We illustrate our approach by studying the conductance of short gold wires that are one atom in diameter. In agreement with recent experiments, we obtain conductance variations with the number of atoms in the wire. Furthermore, the conductance of certain transition metal complexes, that exhibit the Kondo effect, is discussed.

Matthias Ernzerhof obtained his Ph.D. in 1993 from the University of Bonn, Germany. He was awarded a Post-doctoral fellowship from the German Science Foundation to pursue research in density functional theory at Tulane University in New Orleans. In 1998 he took up a position as a senior research scientist in the group of G. Scuseria (Rice University, Houston), where he continued his work in density functional theory. Since 2001 he is assistant professor in theoretical chemistry at the University of Montreal. His present research interests lie in the area of electronic structure theory and molecular electronics.