

Abstract Submitted
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Representing molecules as atomic-scale electrical circuits with fluctuating-charge models JIAHAO CHEN, TODD MARTÍNEZ, University of Illinois at Urbana-Champaign — Fluctuating-charge models (FCMs), also known as chemical potential equilibration models, can describe charge transfer in molecular mechanics (MM). Examples of FCMs are QEq [1], *fluc-q* (FQ) [2], and our recently proposed PE-CC-QVB2 [3] and QTPIE [4]. FCMs describe the accumulation and depletion of atomic charges with electronegativities and chemical hardnesses. We show that this description of atoms maps molecular systems onto electrical circuits. Unlike other models [1, 2], our models correctly model a diatomic molecule in the dissociation limit; we explain how this is reflected in its circuit representation. FCMs hence establish a new connection between the statistical mechanics of molecular electronic structure [5] and classical circuit theory. [1] A. K. Rappe, and W. A. Goddard III, *J. Phys. Chem.* **95**, 3358 (1991). [2] S. W. Rick, S. J. Stuart, and B. J. Berne, *J. Chem. Phys.* **101**, 6141 (1994). [3] J. Morales, and T. J. Martínez, *J. Phys. Chem.* **108A**, 3076 (2004). [4] J. Chen, and T. J. Martínez, *Chem. Phys. Lett.* submitted (2006). [5] J. Morales, and T. J. Martínez, *J. Phys. Chem.* **105A**, 2842 (2001).

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