Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Temperature dependence and anisotropy of charge-carrier mobilities in crystalline durene FRANK ORTMANN, KARSTEN HANNEWALD, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet, Max-Wien-Platz 1, 07743 Jena, Germany — We report on the theoretical analysis of charge-carrier mobilities in durene crystals. The crystal is studied with DFT methods to examine structural, vibrational, and electronic properties. On that basis we employ a Holstein-Peierls model (see Hannewald et al. PRB **69**, 075211 (2004); PRB **69**, 075212 (2004)) to simulate the temperature dependence of the mobilities. The relation between the anisotropy of electron/hole mobilities and the band structure as well as lattice vibrations is discussed.

Frank Ortmann
Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet
Max-Wien-Platz 1, 07743 Jena, Germany

Date submitted: 16 Nov 2006 Electronic form version 1.4