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Dynamical Barrier to Impurity Trapping in Organic Semiconductors DAVID H. DUNLAP, University of New Mexico, PAUL E. PARRIS, Missouri University of Science and Technology, STEPHAN DE BIEVRE, University of Science and Technology, Lille France — We consider the trapping of a moving electron by a polar impurity in an uncompensated organic semiconductor when the multipole moment of the impurity is coupled to an intramolecular vibration, a dynamical generalization of the Vannikov-Novikov dipole trap model.[1] Due to the slow power-law dependence of the multipolar interaction, the vibrational coordinate shifts adiabatically with the approach of the charge carrier. The fast molecular motion can be decoupled from the electron's translational motion to first approximation by transforming to the polaron basis, leading to a polaron binding energy which serves to enhance the propensity for the moving charge to be captured. For an isolated impurity, however, the transformed Hamiltonian contains a repulsive ponderomotive term not described in conventional polaron theory. The repulsion can outweigh the attractive force at long range, presenting a barrier to trap formation. [1] S. V. Novikov and A. V. Vannikov, Chem. Phys. 169 (1993) 21-33.

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