

Supplemental Material:
Effect of Coulomb correlation on charge transport in disordered organic semiconductors

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In this Supplemental Material, a comparison is given between the mobility as studied using ME and KMC simulations as a function of the electric field (Fig. S1), the charge carrier density (Fig. S2) and the relative dielectric constant (Figs. S3 and S4), for sets of simulation parameters that extend those in Figs. 1–3 in the main text. In all figures, the dashed curves give the mobility

as predicted using the parametrization scheme presented in Section III.B. A discussion of the simulation results is given in the last paragraph of Section III.B.

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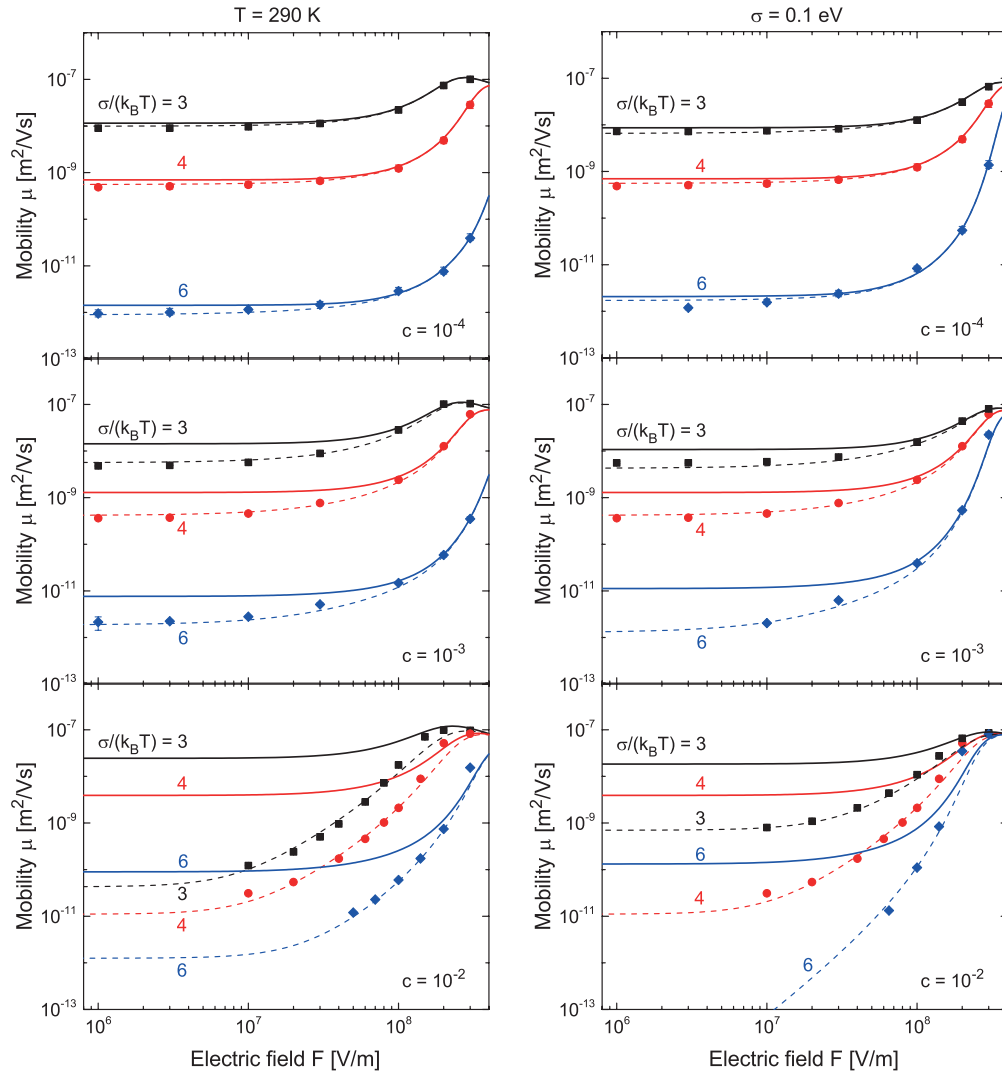


FIG. S1. Calculated charge-carrier mobility μ as a function of the electric field F , at various charge-carrier concentrations c , for various disorder strengths σ at a fixed temperature $T = 290$ K (left) and for various temperatures at a fixed disorder strength $\sigma = 0.1$ eV (right). The three cases studied in each panel correspond to relative disorder strengths $\hat{\sigma} = \sigma/(k_B T)$ equal to 3, 4, and 6. All simulations were performed for $\epsilon_r = 3$. Solid curves: ME results (μ_{ME}). Symbols: KMC results (μ_{KMC}). Dashed curves: μ_{ME} multiplied by the empirical mobility reduction factor given by Eqs. (1)–(3) in the main text.

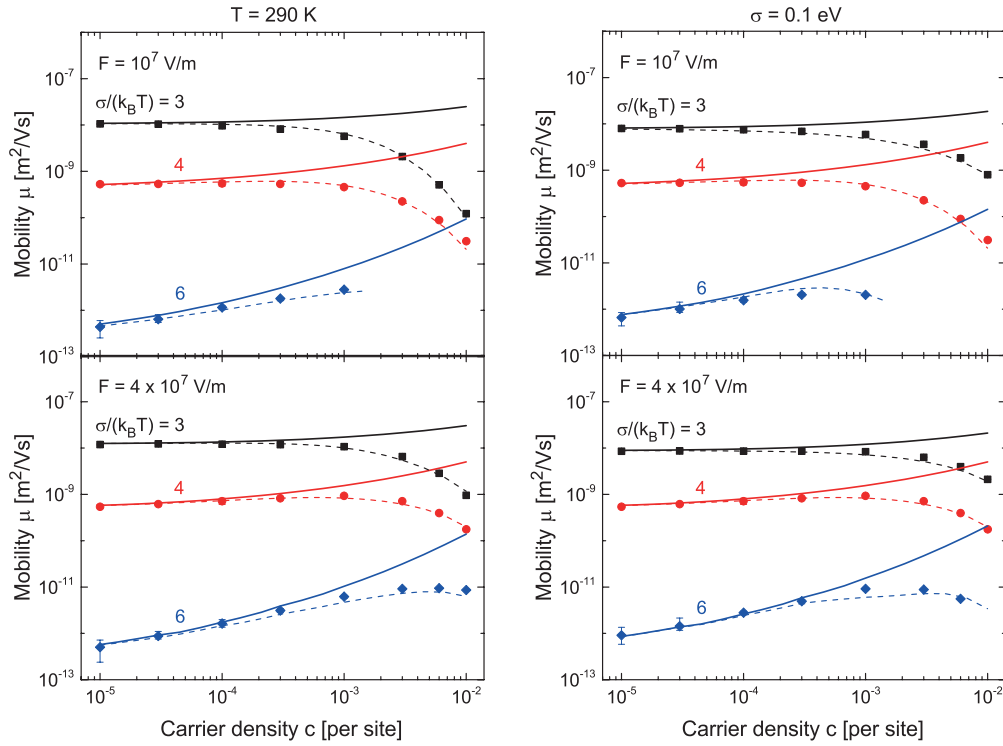


FIG. S2. Calculated charge-carrier mobility μ as a function of the carrier concentration c , for various disorder strengths σ at a fixed temperature $T = 290$ K (left) and for various temperatures at a fixed disorder strength $\sigma = 0.1$ eV (right). The three cases studied in each panel correspond to relative disorder strengths $\hat{\sigma} = \sigma/(k_B T)$ equal to 3, 4, and 6. All simulations were performed for $\epsilon_r = 3$. Solid curves: ME results (μ_{ME}). Symbols: KMC results (μ_{KMC}). Dashed curves: μ_{ME} multiplied by the empirical mobility reduction factor given by Eqs. (1)–(3) in the main text.

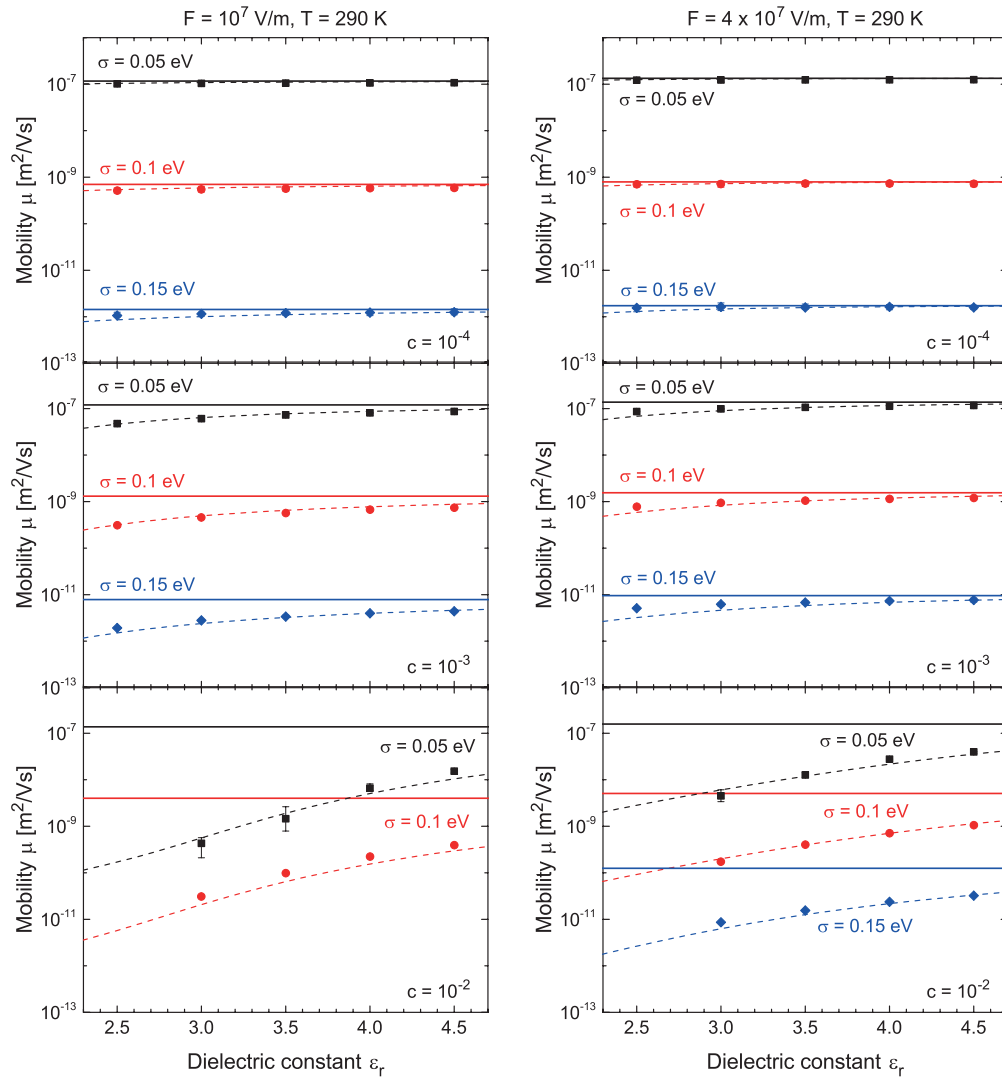


FIG. S3. Calculated charge-carrier mobility μ as a function of the relative dielectric constant ϵ_r at various charge carrier concentrations c and disorder strengths σ , at $F = 10^7$ (left) and $F = 4 \times 10^7$ V/m (right). All simulations were carried out for $T = 290$ K. Solid curves: ME results (μ_{ME}). Symbols: KMC results (μ_{KMC}). Dashed curves: μ_{ME} multiplied by the empirical mobility reduction factor given by Eqs. (1)–(3) in the main text.

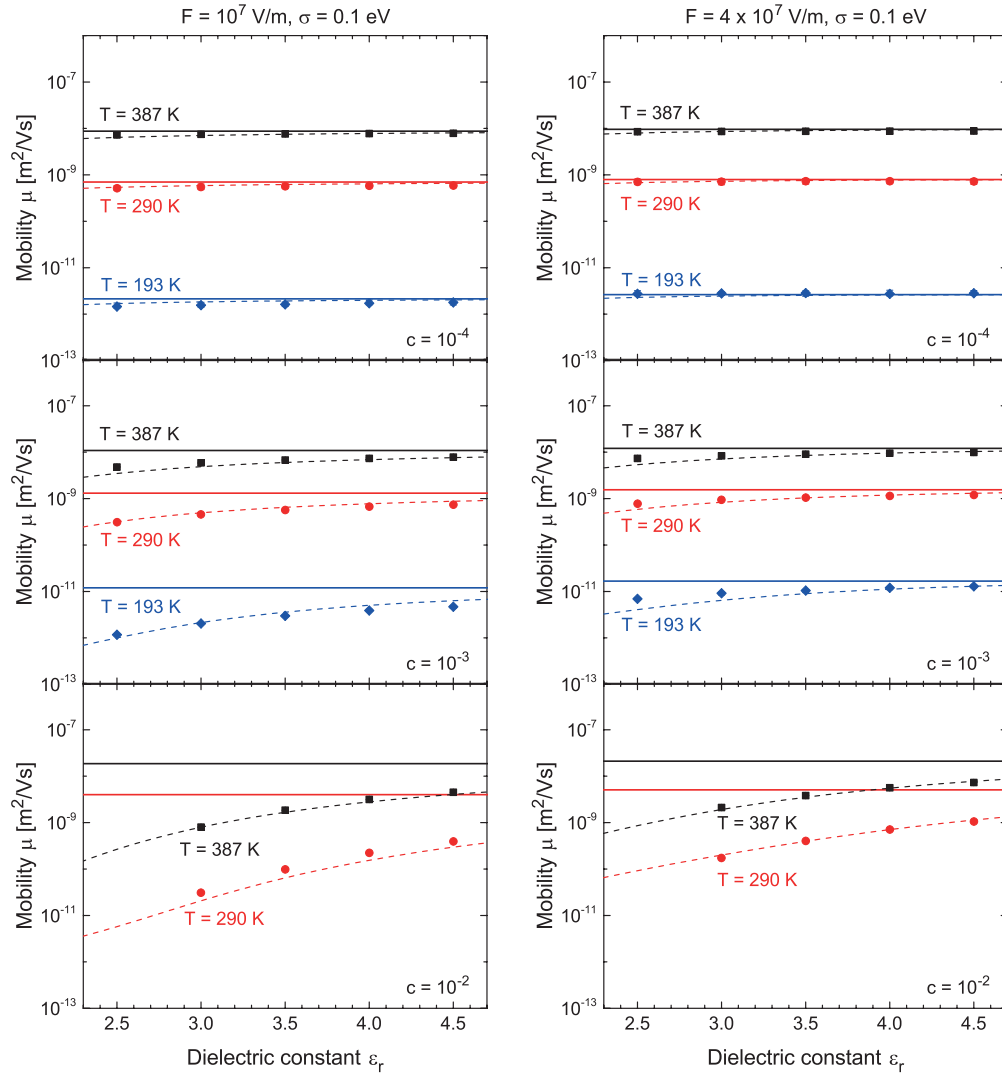


FIG. S4. Calculated charge-carrier mobility μ as a function of the relative dielectric constant ϵ_r at various charge carrier concentrations c and temperatures T , for $F = 10^7$ (left) and $F = 4 \times 10^7$ V/m (right). All simulations were carried out for a fixed disorder strength $\sigma = 0.1$ eV. Solid curves: ME results (μ_{ME}). Symbols: KMC results (μ_{KMC}). Dashed curves: μ_{ME} multiplied by the empirical mobility reduction factor given by Eqs. (1)–(3) in the main text.