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The substitution effect on the reorganization energy of metal free phthalocyanine CHOONGKEUN LEE, KARL SOHLBERG, Department of Chemistry, Drexel University, Philadelphia, Pennsylvania 19104-2875 — Many discotic (disk like) materials such as phthalocyanine are of interest for use in organic electronic devices because of their high charge mobility. The mobility of various discotic materials has been studied using the Marcus formalism. In the Marcus formalism, charge mobility is depends on two parameters, reorganization energy and coupling matrix constant. Of these two parameters the reorganization energy has more influence on the charge hopping rate. A small change in reorganization energy leads to a large change of charge mobility. We have employed electronic structure methods to describe substitution effects on the reorganization energy of phthalocyanine. The substitutions on the external phenyl rings have almost no influence on reorganization energy, but the substitutions on the internal nitrogen in phthalocyanine have strong influence on reorganization energy. The detailed relation between reorganization energy and substitution will be presented.

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