Atomic multipolar contributions to electronic polarization in organic molecular crystals

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Abstract. – The self-consistent computation of electronic polarization in organic molecular crystals is extended to include, in first order, corrections in the continuous gas-phase charge distribution $\rho_{\rm G}(\mathbf{r})$. The potential $\Delta \Phi_a(\mathbf{r}^a)$ at molecule a in the crystal is due to the difference between $\rho_{\rm G}(\mathbf{r})$ and a point-charge approximation. $\Delta \Phi_a(\mathbf{r}^a)$, which represents atomic multipolar contributions, is evaluated for crystals of anthracene and perylenetetracarboxylic dianhydride (PTCDA). The corrections to the polarization energies of molecular cations are $P_+^{(1)} = -0.25$ and $-0.14 \,\mathrm{eV}$ for anthracene and PTCDA, respectively, while $P_-^{(1)} = 0.25$ and $0.18 \,\mathrm{eV}$ for the anions. The leading term of atomic multipoles is the $\Delta \Phi_a(\mathbf{r}^a)$ -charge interaction that corresponds to the charge-quadrupole term in the submolecular approach. There are also new contributions in $\Delta \Phi_a(\mathbf{r}^a)$ -redistributed charge and coupling of induced dipoles to gradients of $\Delta \Phi_a(\mathbf{r}^a)$. First-order correction to electronic polarization is a general approach that combines the advantages of discrete charges for self-consistent treatment of crystals with accurate electrostatic potentials based on the best available molecular charge distribution.

Introduction. – Electronic polarization makes major contributions to ionic states of organic molecular solids, which are typically insulators with low dielectric constants ($\kappa \sim 3$) and small overlap between molecules [1–3]. Molecular exciton theory starts with noninteracting molecules to obtain corrections to gas-phase energies due to the crystalline environment. Such an approach to polarization is more demanding, since corrections to wave functions are required. Electronic polarization is formally the change $\rho(\mathbf{r}) - \rho_{\rm G}(\mathbf{r})$, at fixed atomic positions, between solid and gas-phase charge densities. No general solution is known. Approximate solid-state [4] and quantum-chemical [5, 6] treatments focus on the dielectric properties of semiconductors and molecular polarization, respectively. Small overlap in organic molecular solids suggests another limit, that of zero overlap. Intermolecular forces are then purely electrostatic and the crystal problem in the actual structure reduces to molecules in nonuniform potentials [7]. We have recently presented [7], hereafter I, a self-consistent procedure for electronic polarization in organic molecular crystals based on zero overlap and, in addition, discrete atomic charges, induced dipoles and potentials. We develop here first-order corrections on using $\rho_{\rm G}(\mathbf{r})$ rather than discrete charges. The pronounced advantages of a discrete treatment are the motivation for seeking corrections rather than, for example, attempting a self-consistent continuum analysis.

Electrostatic (Madelung) energies of organic molecular salts are naturally computed using partial charges [8]. The exact charge density $\rho_{\rm G}(\mathbf{r})$ of an isolated (gas-phase) molecular ion is approximated by point charges at atoms to mimic an extended charge distribution. Point atomic charges, which we designate as $\rho^{(0)}(\mathbf{r})$ below and use for neutral molecules, automatically include higher moments of $\rho_{\rm G}(\mathbf{r})$ in part. Electrostatic interactions among neutral molecules lead to multipole expansions with improved convergence on introducing atomic charges and multipoles [9]. In distributed multipolar expansions [10, 11], the potential $\phi_{\rm G}(\mathbf{r}')$ generated by $\rho_{\rm G}(\mathbf{r})$ at points \mathbf{r}' outside the charge distribution is related to atomic charges, dipoles and perhaps quadrupoles that are found by least-squares procedures or optimization on a grid. We instead take $\rho^{(0)}(\mathbf{r})$ from semiempirical theory and associate $\Delta\rho(\mathbf{r}) = \rho_{\rm G}(\mathbf{r}) - \rho^{(0)}(\mathbf{r})$ with the *collective* contribution of atomic multipoles. With the crystal structure as the grid, previous work [10, 11] on $\phi_{\rm G}(\mathbf{r}')$ can readily be applied to electronic polarization in organic crystals.

We consider an organic crystal with Z identical molecules per unit cell and divide the crystal into equal molecular volumes, $V = \sum_{a} V_{a}$. In the approximation of zero overlap, $\rho_{\rm G}^{a}(\mathbf{r})$ of molecule a generates $\phi_{\rm G}^{a}(\mathbf{r}')$ at \mathbf{r}' outside of V_{a} . The electrostatic potential $\Phi_{a}(\mathbf{r}_{a})$ in V_{a} due to all other molecules b is

$$\Phi_a(\boldsymbol{r}^a) = \sum_b' \phi_{\rm G}^b(\boldsymbol{r}^a) = \sum_b' \int_V \mathrm{d}^3 r^b \; \frac{\rho_{\rm G}(\boldsymbol{r}^b)}{|\boldsymbol{r}^a - \boldsymbol{r}^b|}.$$
 (1)

 $\Phi_a(\mathbf{r}^a)$ is the exact *crystal* potential of molecules with *gas-phase* charge distributions and has the crystal's symmetry. We generalize later to lattices with molecular ions at fixed positions. The approximation of $\rho_{\rm G}^a(\mathbf{r})$ as charges $\rho_k^{a(0)}$ at atomic positions \mathbf{r}_k^a is

$$\rho^{a(0)}(\boldsymbol{r}) = \sum_{k} \rho_{k}^{a(0)} \delta(\boldsymbol{r}^{a} - \boldsymbol{r}_{k}^{a}).$$
⁽²⁾

Inserting (2) in (1), we obtain the crystal potential $\Phi_a^{(0)}(\mathbf{r}^a)$ for gas-phase atomic charges. Then $\Delta \Phi_a(\mathbf{r}^a) = \Phi_a(\mathbf{r}^a) - \Phi_a^{(0)}(\mathbf{r}^a)$ is the potential in V_a due to fixed gas-phase $\Delta \rho(\mathbf{r})$. The quadrupole moment of π -electrons is the leading term in $\Delta \rho(\mathbf{r})$ for nonpolar conjugated molecules. Charge-quadrupole corrections to polarization energies in access have been evaluated by Munn [12] using the method of submolecules [2,3].

Electronic polarization requires changes in $\rho_{\rm G}^a(\mathbf{r})$ due to $\Phi_a(\mathbf{r}^a)$, which in turn depends on the charge distribution. Perturbation theory in $\Phi_a(\mathbf{r}^a)$ is not yet practical for large molecules. In solid-state models or semiempirical theory, the discrete potential $\Phi_a(\mathbf{r}_i^a)$ at atom i is a site energy that controls the electron count. Variations of discrete potentials in I yield the atom-atom polarizability tensor Π_{ij} that governs charge flow between atoms i and j. The selfconsistent, discrete solution of electronic polarization in I is based on INDO/S [13] for Π_{ij} and Löwdin atomic charges $\rho_k^{a(0)}$ in (2). The exact polarizability tensor α of an isolated molecule, which in principle follows from $\rho_{\rm G}(\mathbf{r})$, differs from α^C based on INDO/S atomic charges $\rho^{(0)}(\mathbf{r})$. Induced atomic dipoles $\boldsymbol{\mu}_i^a$ are generated by the difference $\tilde{\alpha} = \alpha - \alpha^C = \sum_i \tilde{\alpha}_i$. We obtain self-consistent atomic charges ρ_i^a and induced dipoles $\boldsymbol{\mu}_i^a$ at all \mathbf{r}_i^a in the crystal lattice, and designate the resulting self-consistent potential as $\phi_i^a = \phi_a(\mathbf{r}_i^a)$.

The discrete self-consistent solution neglects $\Delta \rho(\mathbf{r})$ and hence the potential $\Delta \Phi_a(\mathbf{r}^a)$, whose first-order contributions are found below. The central approximation of no intermolecular overlap remains and is also assumed for submolecules [2,3]. In that approach, α is partitioned equally among centers and induced dipoles are found self-consistently. In terms of I, submolecules correspond to $\tilde{\alpha} = \alpha$ and there is no charge redistribution ($\Pi = \alpha^C = 0$).

To first order, we couple the additional potential $\Delta \Phi_a(\mathbf{r}^a)$ to self-consistent charges and dipoles that are not re-optimized. The polarization energy of the lattice changes by

$$E^{(1)} = \sum_{a} \sum_{i} \left(\rho_i^a + \boldsymbol{\mu}_i^a \cdot \nabla \right) \Delta \Phi_a \left(\boldsymbol{r}_i^a \right).$$
(3)

The general expression includes atomic multipoles through $\Delta \Phi_a(\mathbf{r}^a)$ without having to specify individual contributions. We find $\Delta \Phi_a(\mathbf{r}^a)$ in two representative organic molecular crystals. The polarization energy in I is the difference between two extensive quantities, a lattice with ions and a neutral lattice. We evaluate $E^{(1)}$ in both cases to obtain the correction $P_+^{(1)}$ or $P_-^{(1)}$ to the polarization energy of a cation or anion.

Crystal potential of atomic multipoles. – The best-studied organic crystals contain alternant hydrocarbons such as acenes, perylenes, or polyenes [1,2]. The molecules have an inversion center that is often retained in the crystal. The electric field then vanishes by symmetry at the center of mass (c.m.), taken as the origin in (1), and $\Phi_a(0)$ is a saddle point in view of Poisson's equation. More recently, organic devices have focused on perylenetetracarboxylic dianhydride (PTCDA) [14] and α -sexithiophene [15], which have an inversion center but are not alternant. In Hückel theory, alternant hydrocarbons have $\rho_i^{a(0)} = 0$ and the crystal potential (1) is due exclusively to higher moments. Correlated π -electrons in Pariser-Parr-Pople theory also yield $\rho_i^{a(0)} = 0$ in systems with electron-hole symmetry [16]. Small $\rho_i^{(0)}$ are generally found in acenes and the negligible potential (1) based on (2) is then incorrect. In PTCDA, the CO dipoles have substantial $\rho_i^{a(0)}$ and heteroatoms lead to finite atomic charges in general.

To illustrate atomic multipoles, we evaluate $\Phi_a(0)$ and $\Phi_a^{(0)}(0)$ for anthracene [17] and PTCDA [18] crystals. Both have Z = 2 and molecules with c.m. at inversion centers. The molecules are crystallographically equivalent, in contrast to inequivalent pentacenes in that crystal. It is convenient to view (1) for $\Phi_a(\mathbf{r}_i^a)$ as the sum over potentials $\phi_{\rm G}^a(\mathbf{r}_i^b)$ at \mathbf{r}_i^b due to molecule a. Thus $\Phi_a(0)$ is a sum over lattice vectors connecting the c.m.'s. Two sums are needed for pentacene crystals. To evaluate $\Phi_a(\mathbf{r}_i^a)$ at atomic positions, we sum over $\phi_{\rm G}^a(\mathbf{r}_i^b)$ for $b \neq a$. The crystal is an infinite grid that we truncate by choosing M molecules whose c.m. are closest to the origin, so that $M \to \infty$ yields a spherical portion of the infinite crystal. We take Löwdin atomic charges in (2) based on INDO/S and approximate $\rho_{\rm G}(\mathbf{r})$ by density-functional theory (B3LYP) [19] with a substantial basis (6-311++G(d,p)).

The solid lines in fig. 1 depict $\Phi_a(0)$ vs. M in anthracene and PTCDA crystals for the B3LYP charge distribution $\rho_{\rm G}(\mathbf{r})$ of neutral molecules. The dashed lines are $\Phi_a^{(0)}(0)$ for the INDO/S atomic charges, which are indeed negligible for anthracene. All lines become constant by M > 500. Since we have neutral molecules with D_{2h} symmetry, the leading term is the molecular quadrupole. Increasing M adds approximately spherical shells whose contributions vanish, as follows analytically on performing the angular integration over a uniform quadrupole density. Molecular quadrupoles have a divergent, shape-dependent contribution that vanishes for spherical crystals. The potentials in fig. 1 are primarily due to nearby molecules. Atomic multipoles yield corrections of $\Delta \Phi_a^{(0)}(0) = -0.18 \,\mathrm{V}$ in anthracene and $-0.62 \,\mathrm{V}$ in PTCDA. Since a charge q at the origin has energy $q\Delta \Phi_a^{(0)}(0)$, the anthracene result agrees with the charge-quadrupole energy of $-0.168 \,\mathrm{eV}$ for a point charge and submolecules at the ring centers [20].

The correction $E^{(1)}$ in (3) requires $\Delta \Phi_a(\mathbf{r}_i^a)$ at atomic positions. Their *M*-dependencies are similar to fig. 1. We evaluate $\Delta \Phi_a(\mathbf{r}_i^a)$ at M = 1000 for all atoms and show the results



Fig. 1 – Electrostatic potential $\Phi_a(0)$ in anthracene and PTCDA crystals at the center of the molecule at the origin of a spherical cluster of M molecules. Solid lines are based on eq. (1) and densityfunctional theory for $\rho_{\rm G}(\mathbf{r})$. Dashed lines are based on INDO/S atomic charges in eq. (2). The difference $\Delta \Phi_a(0)$ is the collective contribution of higher atomic multipoles.

in fig. 2 as $\Delta \Phi_a(\mathbf{r}_i^a) - \Delta \Phi_a(0)$ for anthracene and PTCDA. The lower symmetry of the crystal potential is evident, with an inversion center at the c.m. instead of D_{2h} symmetry. Negative $\Delta \Phi_a(0)$ leads to negative $\Delta \Phi_a(\mathbf{r}_i^a)$ at atoms *i* in the π -region of either crystal. In



Fig. 2 – Atomic multipolar potential, $\Delta \Phi_a(\boldsymbol{r}_i^a) - \Delta \Phi_a(0)$ in volts, at atom *i* in anthracene and PTCDA crystals. Each molecule has an inversion center.

anthracene, $\Delta \Phi_a(\mathbf{r}^a)$ increases along the long (L) axis and decreases along the medium (M) axis. In PTCDA, $\Delta \Phi_a(\mathbf{r}^a)$ increases along both L and M, but has negative curvature along the normal (N) axis as follows from CO dipoles in the molecular plane. The variations of $\Delta \Phi_a(\mathbf{r}_i^a)$ are small in either case, especially in the central region where atomic charges change on removing or adding a π -electron. The gradients of $\Delta \Phi_a(\mathbf{r}^a)$ are consequently small. They couple in (3) to induced dipoles $\boldsymbol{\mu}_i^a$ that go as $\tilde{\alpha} = \alpha - \alpha^C$ and are ~ 10% corrections to charge redistribution. Although straightforward, the evaluation of three numerical derivatives for the second term of $E^{(1)}$ is lengthy and is a correction to a correction. We evaluate only the larger charge-redistribution terms ρ_i^a in (3).

Polarization correction for molecular ions. – The potential $\Delta \Phi_a(\mathbf{r}_i^a)$ is generated by $\Delta \rho(\mathbf{r}) = \rho_{\rm G}(\mathbf{r}) - \rho^{(0)}(\mathbf{r})$ for a crystal of neutral molecules. The polarization energy P_{\pm} of a molecular cation or anion is found in I as the difference between a lattice with an ion and a neutral lattice. We suppose molecule u to be the ion, with gas-phase charge densities $\rho_{\pm}(\mathbf{r})$ and $\rho_{\pm}^{(0)}(\mathbf{r})$ computed as before. The crystal potential at atoms of a due to gas-phase charges is modified by the ion and (1) becomes

$$\Phi_a^u(\boldsymbol{r}_i^a) = \Phi_a(\boldsymbol{r}_i^a) + (1 - \delta_{au})\Delta\phi_{\rm G}^u(\boldsymbol{r}_i^a).$$
(4)

There is no change at a = u. At other molecules, the change $\Delta \phi_{\rm G}^u$ is the potential due to $\rho_{\pm}(\mathbf{r}) - \rho_{\rm G}(\mathbf{r})$ at u; the leading term is monopolar. A similar expression holds for atomic charges and for $\Delta \Phi_a^u(\mathbf{r}_i^a)$, which is the atomic multipolar contribution when u is a molecular ion. Since point charges are exact for monopoles and approximate for multipoles, $\Delta \Phi_a^u(\mathbf{r}_i^a)$ is entirely due to different atomic multipoles of molecules and molecular ions. Similar $\Delta \rho(\mathbf{r})$ are expected in large molecules and ions whose π -electron count differs by one, and refined electronic structure computations would be needed to obtain reliable differences in anthracene or PTCDA. When such multipolar corrections are neglected, we have $\Delta \Phi_a^u(\mathbf{r}_i^a) = \Delta \Phi_a(\mathbf{r}_i^a)$ and no dependence on the location of the ion.

 $E^{(1)}$ in (3) is a sum over self-consistent atomic charges when the dipole term is neglected. The difference leading to $P_{\pm}^{(1)}$ is a similar sum. The a = u term has ρ_i^{\pm} for the lattice with the ion and $\overline{\rho}_i^u$ for a neutral crystal. The potential is $\Delta \Phi_a(\mathbf{r}^a)$ in either case and gives the largest contribution to $P_{\pm}^{(1)}$,

$$\varepsilon_{\pm}^{(1)} = \sum_{i} \Delta \Phi_u (\boldsymbol{r}_i^u) [\rho_i^{\pm} - \overline{\rho}_i^u].$$
⁽⁵⁾

We obtain $\varepsilon_{+}^{(1)} = -0.27 \,\text{eV}$ for anthracene using self-consistent atomic charges of the cation. The anion correction is $0.28 \,\text{eV}$. The PTCDA results are $\varepsilon_{+}^{(1)} = -0.27 \,\text{eV}$ for the cation and $0.31 \,\text{eV}$ for the anion. Heteroatoms lead to ions with different charge distributions. The $E^{(1)}$ terms with $a \neq u$ in (3) have different multipolar potentials: $\Delta \Phi_a^u(\mathbf{r}_i^a)\rho_i^a$ in the lattice with the ion and $\Delta \Phi_a(\mathbf{r}_i^a)\overline{\rho}_i^a$ in the neutral lattice. In the approximation of unchanged higher multipoles for ion discussed below (4), we have

$$P_{\pm}^{(1)} = \varepsilon_{\pm}^{(1)} + \sum_{i} \Delta \Phi_a(\boldsymbol{r}_i^a) \sum_{a}' \left[\rho_i^a - \overline{\rho}_i^a \right]$$
(6)

for $a \neq u$. The sum represents interactions between higher atomic multipoles and the *total* redistributed charges ρ_i^a at atom *i* of all molecules. The same coefficient $\Delta \Phi_a(\mathbf{r}_i^a)$ appears in (5) and (6), but the self-consistent charges in (5) sum to ± 1 for the ion while those in (6)

sum to zero for molecules. Since $\rho_i^a \to \overline{\rho}_i^a$ far from the ion, contributions of distant sites are negligible and the sum is conveniently evaluated for a sphere of $M \sim 1000$ molecules.

The two terms in (6) have opposite signs for both cations and anions in either anthracene or PTCDA. The first-order correction is $P_{+}^{(1)} = -0.14 \text{ eV}$ for the PTCDA cation and $P_{-}^{(1)} =$ 0.18 eV for the anion. In contrast to acenes [2,3], holes and electrons have different multipolar contributions and a correction of 40 meV appears in the transport gap, which goes as $P_{+} + P_{-}$. The anthracene results are $P_{\pm}^{(1)} = \pm 0.25 \text{ eV}$ for the anion and cation, respectively, and the second term of (6) is a small correction to $\varepsilon_{\pm}^{(1)}$. In π -electron theory, the electron-hole symmetry of anthracene ensures that $\rho_i^a = 0$ in the molecule and $\pm \rho_i^a$ in the ions [16]. The polarization energies of electrons and holes then differ only in sign. Electron-hole symmetry does not apply to all-electron calculations, but its consequences survive whenever π -electrons are a good approximation.

 $P_{\pm}^{(1)}$ is the correction to the self-consistent polarization energy P_{\pm} of a molecular ion found in I. The charge-quadrupole correction [2,3] W_{q-Q} is the submolecular limit of (5). Fixed molecular quadrupoles for anthracene, computed separately and scaled to benzene data, lead to $W_{q-Q} = -0.18 \,\mathrm{eV}$ for charges q/3 at the ring centers [12]. While direct comparisons would require identical α 's, submolecules and charge redistribution clearly yield comparable corrections and the charge-quadrupole interaction is the largest correction in anthracene.

In terms of submolecules, the second term of (6) corresponds to interactions between induced dipoles and higher multipoles that, to our knowledge, have not been evaluated previously. Multipole–induced-dipole interactions are small in anthracene and presumably in other accens, but they are substantial in PTCDA, about half of the multipole-charge term.

The treatment of electronic polarization in I holds for organic molecular crystals in general when intermolecular overlap is neglected and yields self-consistent results for discrete atomic charges and potentials. Experimental comparisons to date are to the optical dielectric tensors of anthracene and PTCDA [21]. The procedure is applicable to crystalline thin films and accounts for the variation of the PTCDA transport gap, E_t , with film thickness on gold or silver substrates [22]. Since E_t goes as $P_+ + P_-$, multipolar corrections cancel in acenes as found previously using submolecules [1, 2], but not in PTCDA or other molecules with heteroatoms. The transport states of crystalline thin films are critical for electronic organic devices that depend on currents, electronic polarizations at surfaces and interfaces provide many applications. Theoretical comparisons to submolecular results for P_+ , P_- and the binding energy $V(\mathbf{r})$ of a cation-anion pair at separations \mathbf{r} are discussed in I. The agreement is best with the choice of the largest number of submolecules. With discrete atomic charges and potentials, the self-consistent computation of charge redistributions becomes practical. Firstorder corrections to polarization energies due to atomic multipoles can also be found in general.

In summary, the correction $E^{(1)}$ in (3) includes atomic multipole contributions to electronic polarization found self-consistently using discrete atomic charges, induced dipoles and potentials in molecular crystals with zero intermolecular overlap. All higher multipoles are included in $\Delta \Phi_a(\mathbf{r}^a)$, which is seen in fig. 2 to be a slowly varying potential in crystalline anthracene and PTCDA. The correction $P_{\pm}^{(1)}$ is $\pm 0.25 \,\mathrm{eV}$ for an anthracene anion and cation, respectively, $-0.14 \,\mathrm{eV}$ for PTCDA⁺ and $0.18 \,\mathrm{eV}$ for PTCDA⁻.

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