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Supporting information for article:

Lattice defects in quinacridone

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Supporting information 1. Cif files of the structural models

The following structures are electronically available as cif files in the supporting material:

- Experimental structure of αI-quinacridone, in the unit cell setting used for the simulation of lattice defects (without lattice defects, before lattice-energy minimisation)
- Twin model 1
- Layer misfit structure

Cif files of all other models are available from the corresponding author upon request.

2. Force field evaluation

Table S1  Evaluation of the force field, using the four polymorphic structures of quinacridone. Dreiding calculations were performed with ESP charges and Ewald summation. Lattice energies are reported in kJ/mol, relative to the αI-phase.

| Phase       | αI | αII | β   | γ    |
|-------------|----|-----|-----|------|
| Erel (Dreiding) | 0  | 1.5333 | -2.3407 | -6.4931 |
| Erel (DFT-D)   | 0  | -1.0869 | -5.2935 | -6.5214 |

Table S2  Evaluation of the force-field: Lattice-energy optimiziation on αII-, β-, and γ-quinacridone without lattice defects.

| αII-Phase | Experimental | Dreiding | DFT-D |
|-----------|--------------|----------|-------|
| a / Å     | 7.0500       | 6.9106   | 6.797 |
| b / Å     | 28.4000      | 29.4171  | 28.532 |
| c / Å     | 3.9000       | 3.9058   | 3.699 |
| α / °     | 90.0000      | 90.0000  | 90.000 |
| β / °     | 110.0000     | 117.1972 | 111.909 |
| γ / °     | 90.0000      | 90.0000  | 90.000 |
### Supporting information, sup-2

|   |   |   |   |
|---|---|---|---|
| $V / \text{Å}^3$ | 733.767 | 706.223 | 682.385 |
| $\beta$-Phase | Experimental | Dreiding | DFT-D |
| $a / \text{Å}$ | 5.692(1) | 5.7373 | 5.775 |
| $b / \text{Å}$ | 3.975(1) | 3.9482 | 3.724 |
| $c / \text{Å}$ | 30.02(4) | 30.3105 | 29.570 |
| $\alpha / ^\circ$ | 90.00 | 90.0000 | 90.000 |
| $\beta / ^\circ$ | 96.76(6) | 96.8244 | 96.598 |
| $\gamma / ^\circ$ | 90.00 | 90.0000 | 90.000 |
| $V / \text{Å}^3$ | 674.502 | 681.729 | 627.539 |
| $\gamma$-Phase | Experimental | Dreiding | DFT-D |
| $a / \text{Å}$ | 13.697(9) | 14.0823 | 13.407 |
| $b / \text{Å}$ | 3.881(3) | 3.8538 | 3.747 |
| $c / \text{Å}$ | 13.4020(10) | 13.5430 | 13.065 |
| $\alpha / ^\circ$ | 90.00 | 90.0000 | 90.000 |
| $\beta / ^\circ$ | 100.44(1) | 100.6366 | 98.244 |
| $\gamma / ^\circ$ | 90.00 | 90.0000 | 90.000 |
| $V / \text{Å}^3$ | 700.63 | 722.355 | 649.551 |

### 3. Model with lamellar domains with misoriented molecules

Table S3: Lattice parameters of the model of the lamellar domains with misoriented molecules, and of the undisturbed unit cell.

|   | Lamellar domain | Unit cell |
|---|---|---|
| $a / \text{Å}$ | 3.8402 | 3.9241 |
| $b / \text{Å}$ | 6.8962 | 6.8938 |
| $c / \text{Å}$ | 8 * 15.1071 | 14.9598 |
| $\alpha / ^\circ$ | 99.864 | 98.999 |
| $\beta / ^\circ$ | 97.700 | 100.601 |
| $\gamma / ^\circ$ | 115.269 | 114.976 |