Supplementary Information

Crystal Phase Transition of Urea: What Governs the Reaction Kinetics in Molecular Crystal Phase Transition

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1. Other crystal structures for urea

In Fig. S1, we show further 8 urea crystal structures, including phase IV and III mentioned in the manuscript (Crystal A to C are shown in Fig. 2) and crystal D, E, F, G, H and J that are within 1 kcal/mol per molecule from the GM (calculated by DFT). The properties of Crystal D, E, F, G, H and J are summarized in Table S1.

Table S1: Six metastable crystal structures of urea.

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| H     | P2
| J     | P2_1/c | 77.3 | 2 (III)    | 0.79 |

*Listed data includes the symmetry group (S.G.), the volume (Å³/mole.), the average number of H-bond per molecule (N_{H-bond}) and the relative energy (E) with reference to the GM (phase III). All
energies are in the unit of kcal/mol per molecule.

*Roman number in parenthesis describes the H\textsubscript{bond} network pattern in Fig. 1 of the manuscript.

**Figure S1**: Crystal structures of low energy urea crystals. The 12 crystals are labelled in the upper left global PES.
2. Barriers to transform to crystal A that calculated using Amber force field.

Table S2: Barriers to transform to crystal A that calculated using Amber force field.

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3. Pathway for the transformation from crystal C to B

Crystal C has a different hydrogen network (only Type-III) from the other low energy crystal structures (generally containing Type-I network), and thus has been found to have a high barrier to transit to other low energy crystals (see Fig. 3). In Figure S2, we show the reaction snapshots in the lowest energy pathway from crystal C to B. We noticed that a large atomic movement are required in the reaction, where 50% $H_{bond}$ in Crystal C breaks at the TS (Fig. S2). The barrier of the transformation is 2.24 kcal/mol per molecule (Fig. 3).
**Figure S2:** Reaction snapshots from Crystal B to C in the lowest energy pathway. Two view angles, [001] and [010] with reference to crystal D lattice, are shown.
4. PES of 16 urea molecules per unit cell.

We have also done a SSW search based on urea crystals with 16 molecules per unit cell. $10^5$ minima are visited in total in 10 parallel runs. The main features of the PES obtained from 8-molecule crystals are reserved in this figure, including the solid-liquid boundary at 1.5 kcal/mol and many solid phases along the OP$_d$=1.0 region. Due to system scale, less crystal phases are observed within $10^5$ steps, making this figure sparse compare to Fig. 2b in the manuscript.

![Figure S3](image.png)

Figure S3. The PES of urea crystals with 16 molecules per unit cell.

5. Structure information for urea crystal structures in .arc format.

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S-12
Crystal J

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