

Supporting Information

EpiCalc epitaxy calculation for the (001) faces of Form II acetaminophen and graphite

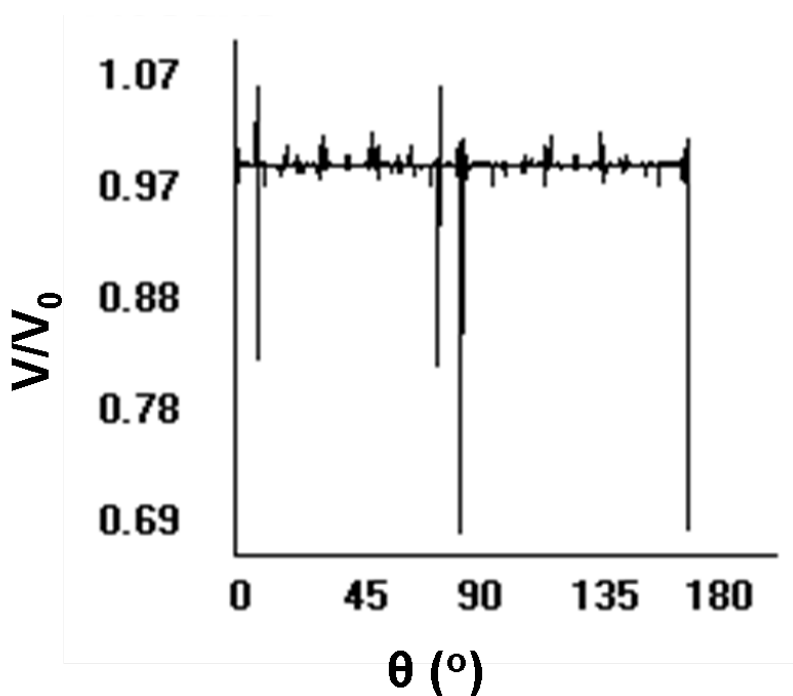


Figure S1. A plot of dimensionless potential energy (V/V_0) as a function of orientation angle (θ) for the interacting (001) faces of Form II acetaminophen and graphite

The EpiCalc calculation was performed using the following lattice values for the (001) faces of Form II acetaminophen and graphite:

(001) Form II acetaminophen: $a = 17.1657 \text{ \AA}$, $b = 11.7773 \text{ \AA}$ and $\beta = 90^\circ$

(001) graphite: $a = b = 2.456 \text{ \AA}$ and $\alpha = 90^\circ$

The acetaminophen overlayer dimensions were 25×25 cells and the orientation angle range tested was 180° with a step size of 0.25° .

Figure S1 shows that the minimum value of $V/V_0 = 0.6861$ when $\theta = 0$ and 90° .