In order to implement the results into the PN mode, we fit the results using a Fourier series that reflects the lattice symmetry of the basal plane of the *hcp* structure: $\gamma(\vec{\delta}) = \sum_{\vec{\mathbf{G}}} c_{\vec{\mathbf{G}}} \exp(i\tilde{\mathbf{G}} \cdot \vec{\delta})$, in which we use a set of 81 two-dimensional reciprocal lattice vectors $\tilde{\mathbf{G}}$. The results are shown in Fig. 2. The perfect crystal configuration, which has GSF value of zero, is associated with the displacement $\vec{\delta} = 0$ and its periodic equivalents. The ISF configuration, which corresponds to the displacement vector (and equivalents) $\vec{\delta} = (0,\, b_p)$, with $b_p = \frac{1}{3}\sqrt{3}a = 2.0996$ Å the length of a partial Burgers vector, has an excess energy of 0.0063 mJ/m^2.

Using our estimates for the elastic properties and the GSF surface in the PN model, we investigate the structure and intrinsic mobility of 4 dislocation types on the basal plane: (i) screw, (ii) 30°, (iii) 60°, and (iv) edge. Fig. 3 shows the optimized disregistry profile for the screw dislocation, obtained by minimizing Eq. (1) at zero external stress. As expected, given the low stacking-fault energy (SFE) value , it dissociates into two 30°partial dislocations with opposite edge components, separated by an ISF area with a width of 29 atomic rows, which corresponds to 91.33 Å. The core width ς of the partials, defined as the distance over which the displacement changes from $\frac{1}{4}$ to $\frac{3}{4}$ of it total value[14], is approximately 1 atomic row or ∼3.1 Å. The second line of Table II contains the dissociation widths of the other three dislocations, showing an increasing ISF width with increasing edge component, consistent with dislocation theory [1].

In addition to the structural properties described here, the PN model permits an estimate of the intrinsic dislocation mobility, which is measured in terms of the Peierls stress. To this end, we impose an external shear stress in the glide plane parallel to the total Burgers vector. It produces maximal force per unit length [1] on the dislocation line for the given stress magnitude. This magnitude is then increased in small steps, followed by minimization of Eq. (1) with respect to the disregistry vectors $\vec{\delta_i}$. At a critical stress value, the so-called Peierls stress, an instability is reached and an equilibrium solution ceases to exist.[14, 15] In this situation the dislocation becomes free to move through the crystal. The third line of Table II contains the Peierls stress values for the four considered dislocation types. The lowest Peierls stress value, obtained for the 30° dislocation, is of the order of 1.5×10^{-2} MPa. This value is ∼ 3 orders of magnitude smaller than the shear modulus, which is consistent with the typical discrepancy between the ideal shear strength and actual yield stresses in crystals [1].