Nanotubes Motion on Layered Materials: A Registry Perspective

Supplementary Information

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Replacing atomic centered circle overlaps by projected Gaussian overlaps

In the original implementation of the registry index method atomic centered circles were used to evaluate the degree of inter-lattice commensurability at rigid interfaces. This choice allowed the efficient evaluation of projected circle overlaps via a simple analytic expression. Notably, this simplistic picture was able to rationalize the measured frictional behavior of a bilayer graphene junction.[1,2] Nevertheless, the obtained RI surfaces were characterized by somewhat sharp features when compared to the corresponding sliding energy landscapes calculated using advanced first-principles method.[3] In order to obtain smoother and more physical RI surfaces that better match the reference calculations we have replaced the atomic centered circles by two-dimensional Gaussians. The latter provide a softer reduction of the projected pair overlaps as a function of lateral inter-atomic distance (see Fig. S1) while maintaining the analytic nature of the overlap area evaluation.

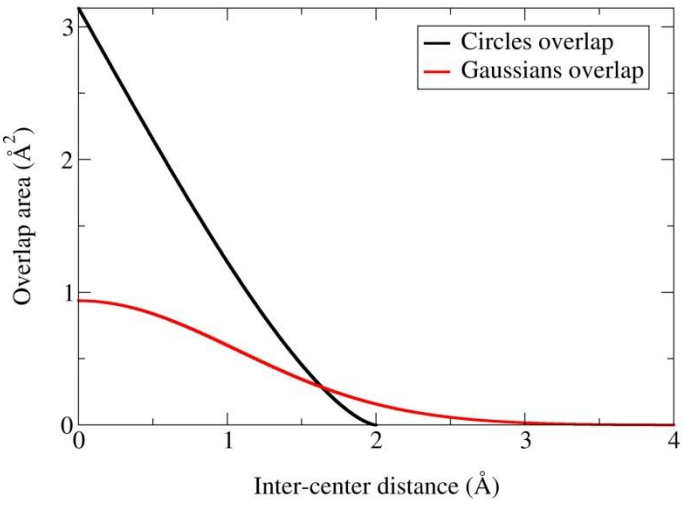

Figure S1: Circle vs. Gaussian pair overlap. Comparison of the pair overlap of two circles (black) and two Gaussians (red) as a function of their inter-center distance, d. The pair circle overlaps are calculated using $S_{ij}^{circle} = \mathrm{r_i^2}\cos^{-1}\left[\left(\mathrm{d^2} + \mathrm{r_i^2} - \mathrm{r_j^2}\right)/(2\mathrm{dr_i})\right]$ $+\mathrm{r_j^2}\cos^{-1}\left[\left(\mathrm{d^2} + \mathrm{r_j^2} - \mathrm{r_i^2}\right)/(2\mathrm{dr_j})\right] - 0.5\sqrt{(\mathrm{r_i} + \mathrm{r_j} - d)(\mathrm{r_i} - \mathrm{r_j} + d)(\mathrm{r_j} - \mathrm{r_i} + d)(\mathrm{r_i} + \mathrm{r_j} + d)}$, where $\mathrm{r_i} = \mathrm{r_j} = 1$ Å are the two circle radii. The pair Gaussian overlaps are calculated using $S_{ij}^{Gaussian} = \left(\pi\sigma_i^2\sigma_j^2/\sqrt{\sigma_i^2 + \sigma_j^2}\right)e^{-0.5d^2/\left(\sigma_i^2+\sigma_j^2\right)}$ with $\sigma_i = \sigma_j = 0.75$ Å being the Gaussian standard deviations.

To demonstrate the performance of the new implementation we compare, in Fig. S2, the sliding RI surface of periodic bilayer *h*-BN obtained using circle (left panel) and Gaussian (middle panel) overlaps with the corresponding sliding energy landscape (right panel) obtained using the TS-vdW dispersion corrected PBE exchange-correlation density functional approximation with the tier-2 basis set of the FHI-AIMS code given in Ref. [3]. As can be seen, the RI landscape obtained using Gaussian overlaps is in good agreement with the reference DFT results providing a better physical picture than the corresponding circle overlap based calculation without any increase in computational cost or complexity.

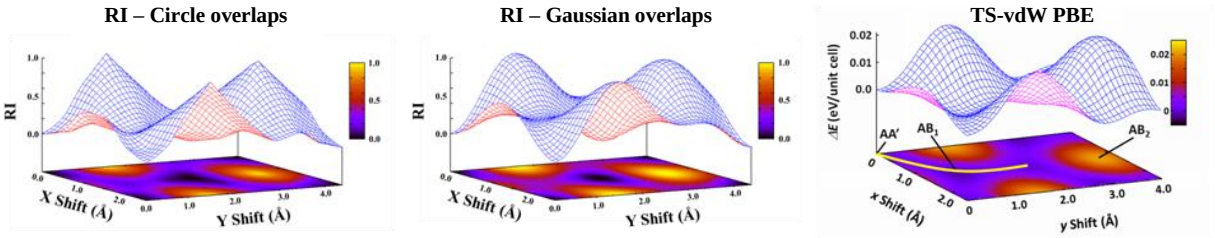

Figure S2: Circle vs. Gaussian overlap sliding RI landscapes. Comparison of sliding RI landscapes obtained using circle overlaps (left panel) and Gaussian overlaps (middle panel) with the reference sliding energy calculations of bilayer *h*-BN (right panel) obtained using the TS-vdW dispersion corrected PBE exchange-correlation density functional approximation and the tier-2 basis set as implemented in the FHI-AIMS code.[3] The circle radii used are $\mathrm{r_N} = 0.5\mathrm{a_{BN}}$ and $\mathrm{r_B} = 0.15\mathrm{a_{BN}}$ with $\mathrm{a_{BN}} = 1.446$ Å being the equilibrium BN bond length in *h*-BN. Gaussian standard deviations are given by $\sigma_N = 0.75\mathrm{r_N}$ and $\sigma_B = 0.75\mathrm{r_B}$.

Anisotropic pair-overlap registry index calculation

When calculating the nanotube/substrate atomic centered Gaussian overlaps within the registry index method curvature effects should be taken into account. To do so we follow the Kolmogorov-Crespi[4] and *h*-BN ILP[5] approach. In these methods the inter-layer interactions depend on the lateral distance ρ_{in} (see Fig. S3) between atoms *i* and *n* on adjacent layers. ρ_{in} is defined as the distance between atom *n* of one layer and the surface normal at the position of atom *i* of the other layer. The latter is taken as the normal to the surface defined by the three nearest-neighbors of atom *i* within the hexagonal lattice.

In the original implementation of the registry index method for flat parallel surfaces, the circle overlaps were calculated as a function of the lateral distance $\rho_{in} = \rho_{ni}$ between each pair of atoms (*i* and *n*) in adjacent layers. When considering non-parallel surfaces the lateral distance is no longer symmetric such that $\rho_{in} \neq \rho_{ni}$. To account for this, the Gaussian pair overlap is taken as the average of the overlap calculated using ρ_{in} and ρ_{ni} in the following manner:

$$S_{in} = 0.5 \cdot [S(\rho_{in}) + S(\rho_{ni})], \quad (1)$$

where $S(\rho_{in})$ and $S(\rho_{ni})$ are the Gaussian overlaps of atoms *i* and *n* calculated using Eq. 1 of the main text at lateral distances ρ_{in} and ρ_{ni}, respectively, and S_{in} is the average overlap area of the atomic pair. With this definition the overlap becomes dependent on the relative spatial orientation of the two 2D-Gaussians and reduces with increasing inter-Gaussian tilt angle.

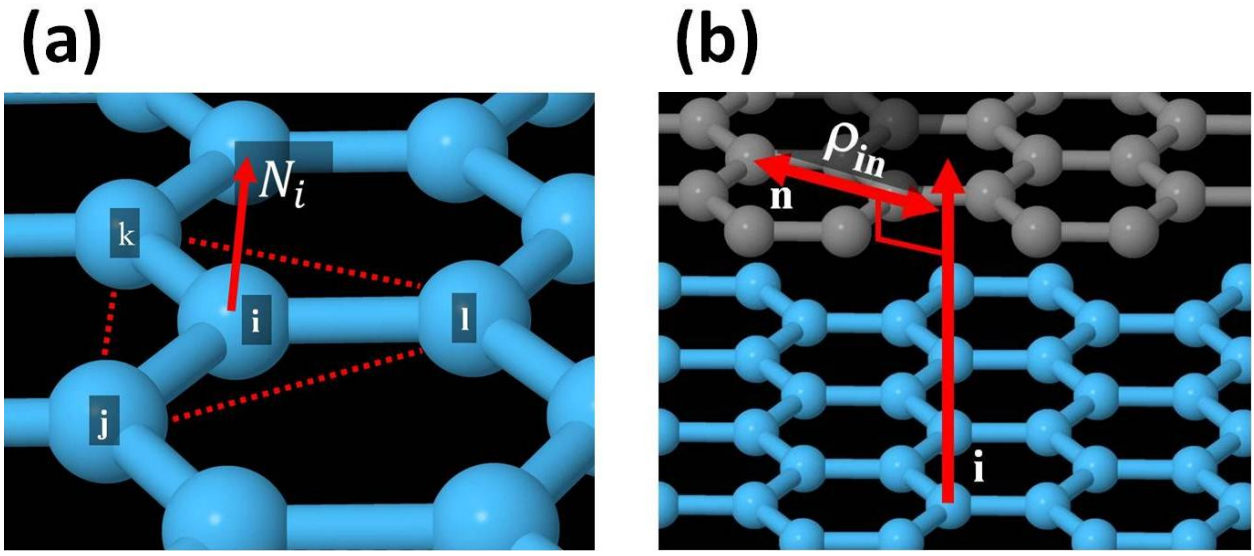

Figure S3: Normal and lateral inter-atomic distance definitions. (a) The surface normal at the position of atom *i*, N_i, is defined as the normal to the plane defined by its three nearest-neighbors *j*, *k* and *l*. (b) The lateral distance ρ_{in} is the shortest distance between atom *n* of one layer and the normal of atom *i*. For clarity we show here a bilayer graphene system and color the lower layer atoms in cyan.

References

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