

Critical size for molecule-to-bulk transition in 2D structure

(Supplementary materials)

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The following are included as supporting information for this paper:

Total 4 Pages, 6 Tables.

Table S1. The average area of inner units (S_{in}) and outermost units (S_{out}) in graphene and their difference(ΔS) with corresponding radius(R) of graphene.

$R(\text{nm})$	$S_{in}(\text{\AA}^2)$	$S_{out}(\text{\AA}^2)$	$\Delta S(\text{\AA}^2)$
0.3409	5.2934	5.2020	0.0914
0.5631	5.2646	5.2313	0.0333
0.7866	5.2593	5.2464	0.0128
1.0105	5.2599	5.2578	0.0021
1.2345	5.2599	5.2632	-0.0033
1.4586	5.2613	5.2670	-0.0057
1.6828	5.2626	5.2695	-0.0069
1.9070	5.2635	5.2708	-0.0073
2.1313	5.2642	5.2719	-0.0077
2.3555	5.2646	5.2716	-0.0070

Table S2. The average area of inner units (S_{in}) and outermost units (S_{out}) in h -BN and their difference(ΔS) with corresponding radius(R) of h -BN.

$R(\text{nm})$	$S_{in}(\text{\AA}^2)$	$S_{out}(\text{\AA}^2)$	$\Delta S(\text{\AA}^2)$
0.3476	5.4558	5.4161	0.0397
0.5734	5.4507	5.4270	0.0237
0.8004	5.4492	5.4302	0.0190
1.0279	5.4485	5.4318	0.0167
1.2556	5.4476	5.4323	0.0153
1.4834	5.4478	5.4331	0.0147
1.7113	5.4478	5.4335	0.0143
1.9392	5.4474	5.4336	0.0137
2.1671	5.4471	5.4337	0.0134

Table S3. The average area of inner units (S_{in}) and outermost units (S_{out}) in two-dimensional siligraphene and their difference(ΔS) with corresponding radius(R) of two-dimensional siligraphene.

$R(\text{nm})$	$S_{in}(\text{\AA}^2)$	$S_{out}(\text{\AA}^2)$	$\Delta S(\text{\AA}^2)$
0.4879	8.3484	8.3062	0.0422
0.8143	8.3494	8.3235	0.0259
1.1402	8.3458	8.3231	0.0227
1.4660	8.3434	8.3223	0.0211
1.7917	8.3412	8.3212	0.0200
2.1174	8.3398	8.3201	0.0197

Table S4. The average area of inner units (S_{in}) and outermost units (S_{out}) in planar MgO and their difference(ΔS) with corresponding radius(R) of planar MgO.

$R(\text{nm})$	$S_{in}(\text{\AA}^2)$	$S_{out}(\text{\AA}^2)$	$\Delta S(\text{\AA}^2)$
0.3310	3.7056	3.8401	-0.1345
0.5554	3.8722	3.8796	-0.0074
0.7802	3.9050	3.9012	0.0038
1.0053	3.9225	3.9154	0.0071
1.2305	3.9346	3.9243	0.0103

Table S5. The average area of inner units (S_{in}) and outermost units (S_{out}) in planar LiF and their difference(ΔS) with corresponding radius(R) of planar LiF.

$R(\text{nm})$	$S_{in}(\text{\AA}^2)$	$S_{out}(\text{\AA}^2)$	$\Delta S(\text{\AA}^2)$
0.3092	3.2471	3.3493	-0.1022
0.5202	3.4021	3.3995	0.0026
0.7314	3.4372	3.4223	0.0149
0.9431	3.4565	3.4386	0.0179
1.1547	3.4688	3.4484	0.0204

Table S6. The critical size of five two dimensional materials.

System name	Critical size(nm)
graphene	1.9070
<i>h</i> -BN	1.7113
two-dimensional siligraphene	1.1402
planar MgO	0.7802
planar LiF	0.7314