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Supporting information: Towards an accurate description of one-dimensional pnictogen allotropes in nano-confinement

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Fig. S1-S4: additional plots of energies. Fig. S5: tests on the influence of axial position on the binding energy. Fig. S6-S8: plots of RDCP potential. Table S1-S12: energy data.

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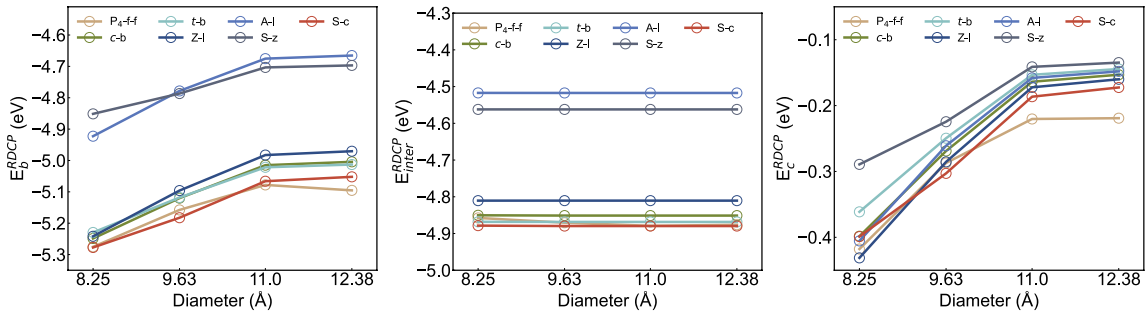

FIG. S1. The binding energy of P as a function of confinement size. (a) The total binding energy under RDCP, without applying segment corrections. (b) The inter-atomic interaction energy under RDCP. (c) The confining interaction of segment under RDCP.

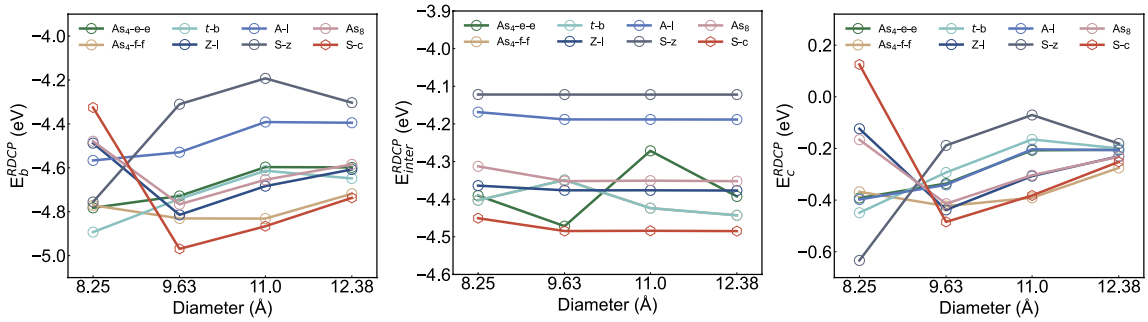

FIG. S2. The binding energy of As as a function of confinement size. (a) The total binding energy under RDCP, without applying segment corrections. (b) The inter-atomic interaction energy under RDCP. (c) The confining interaction of segment under RDCP.

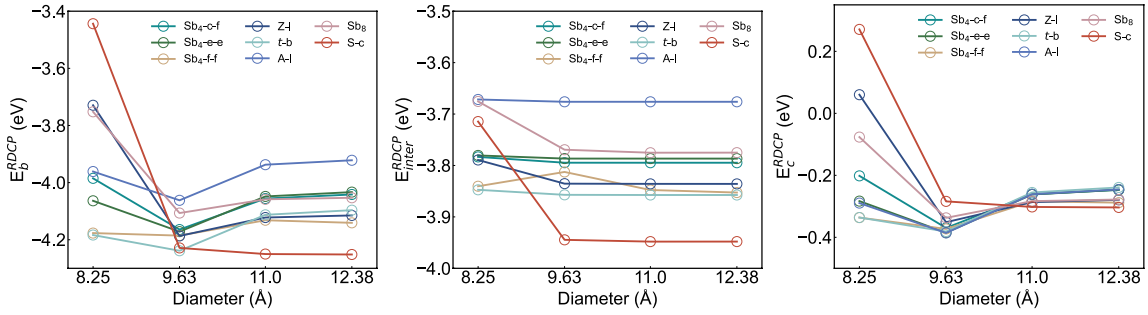

FIG. S3. The binding energy of Sb as a function of confinement size. (a) The total binding energy under RDCP, without applying segment corrections. (b) The inter-atomic interaction energy under RDCP. (c) The confining interaction of segment under RDCP.

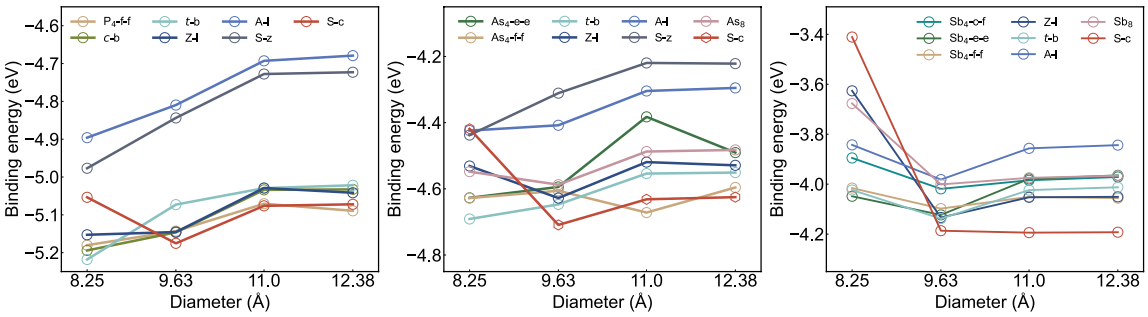

FIG. S4. The RDCP-DFT calculations of the binding energy of P (a), As (b) and Sb (c), using segment correction terms calculated by the SCAN exchange correlation functional.

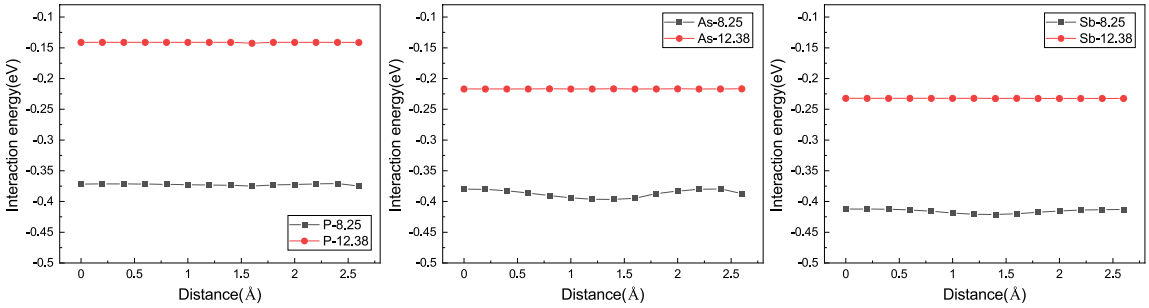

FIG. S5. The influence of positions of segments in the axial dimension on the confining interaction energy. The test calculations are performed on the 8-atom ladder structure, which is used for the RDCP training. The structure is placed in the middle of the 8.25 Å and the 12.38 Å carbon nanotubes. The interaction energy is plotted as a function of the distance moved in the axial dimension. The tests show that the influence of axial position on the interaction energy is negligible compared to the other factors.

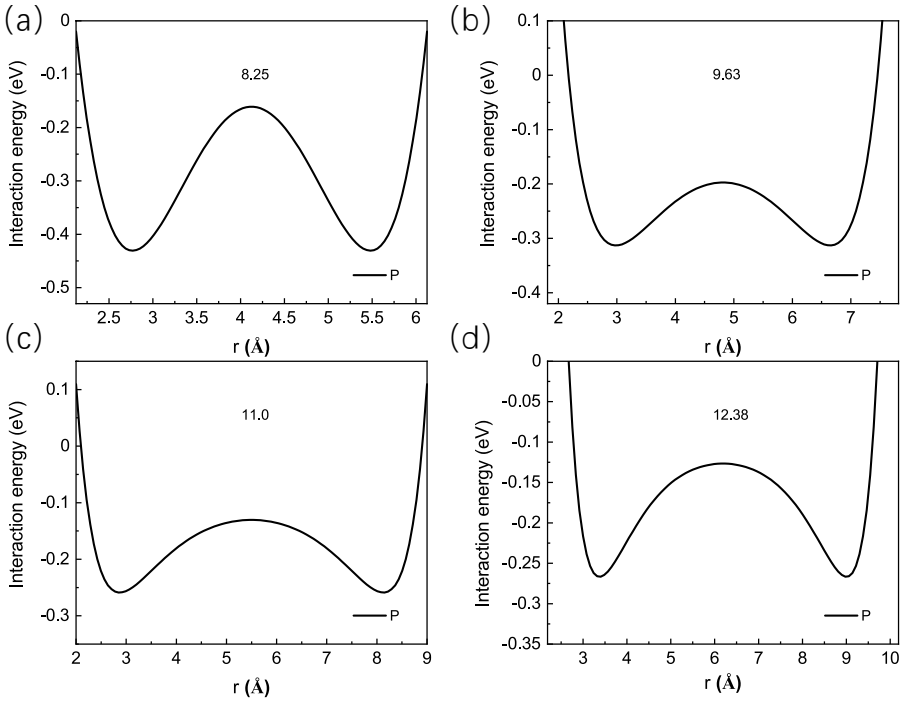

FIG. S6. The RDCP confining interaction energy of P as a function of the r in different confinement size (diameter).

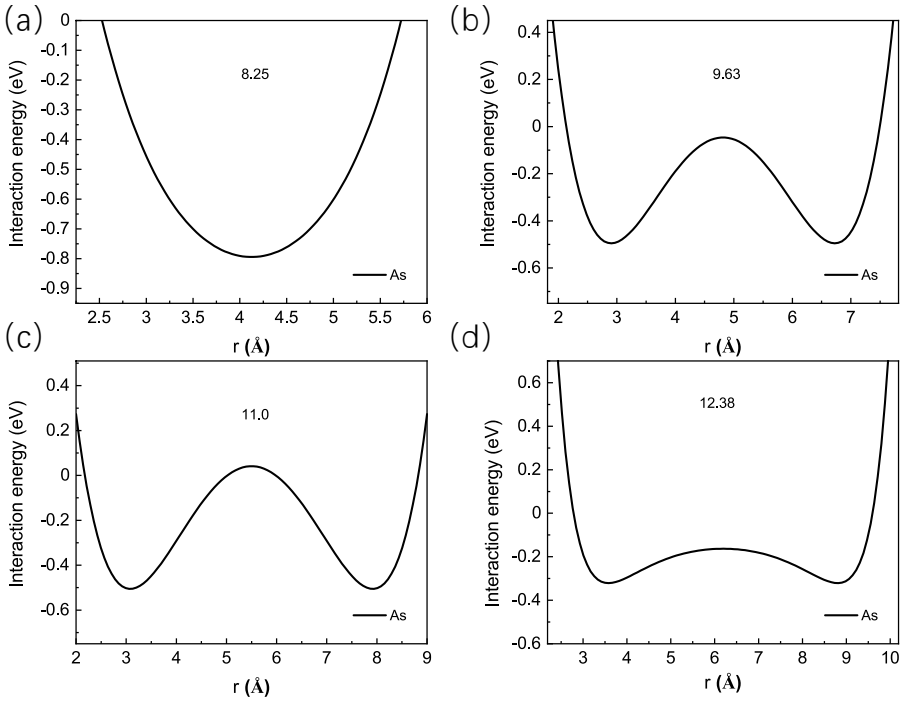

FIG. S7. The RDCP confining interaction energy of As as a function of the r in different confinement size (diameter).

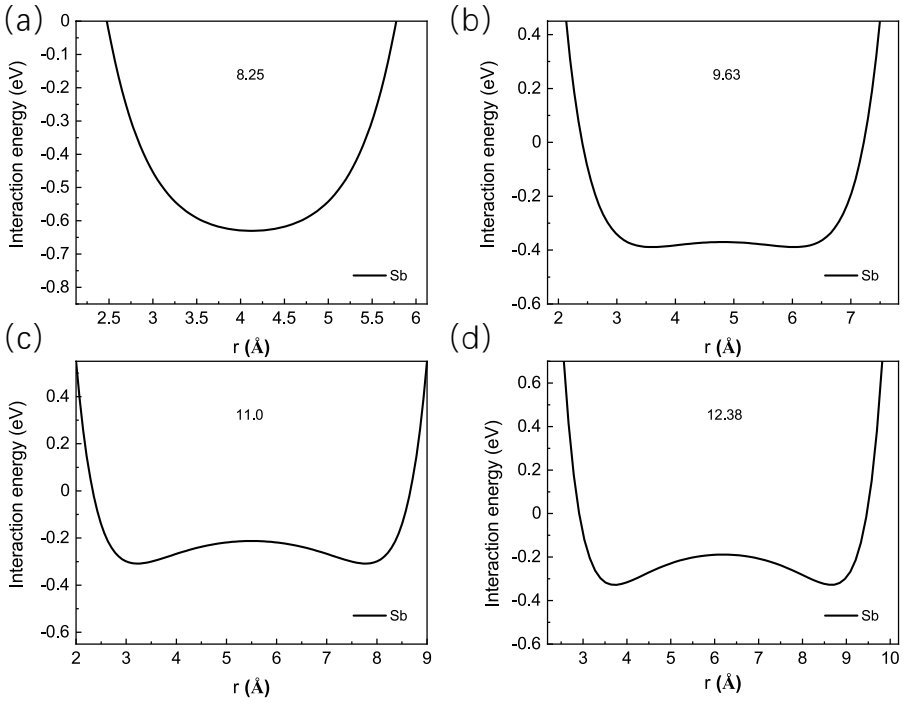

FIG. S8. The RDCP confining interaction energy of Sb as a function of the r in different confinement size (diameter).

$2R$=8.25 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-face-face	-5.27534	-4.85756	-0.32267	-0.41778	-5.18023
cis-butterfly	-5.24871	-4.85036	-0.34376	-0.39835	-5.19413
trans-butterfly	-5.22953	-4.86822	-0.34982	-0.36131	-5.21803
zigzag-ladder	-5.24172	-4.81049	-0.34221	-0.43123	-5.1527
alternating-ladder	-4.92263	-4.51717	-0.3788	-0.40546	-4.89596
single-zigzag	-4.85136	-4.56208	-0.41475	-0.28928	-4.97684
square-columnar	-5.27742	-4.87852	-0.17508	-0.3989	-5.0536

TABLE S1. Table for P under 8.25 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=9.63 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-face-face	-5.15769	-4.87053	-0.27253	-0.28716	-5.14306
cis-butterfly	-5.1201	-4.85114	-0.29522	-0.26896	-5.14636
trans-butterfly	-5.11802	-4.86844	-0.20451	-0.24958	-5.07295
zigzag-ladder	-5.09593	-4.81046	-0.33498	-0.28547	-5.14544
alternating-ladder	-4.77829	-4.51729	-0.29238	-0.261	-4.80967
single-zigzag	-4.78662	-4.56213	-0.28162	-0.22449	-4.84375
square-columnar	-5.18255	-4.87964	-0.29569	-0.30291	-5.17532

TABLE S2. Table for P under 9.63 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=11.0 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-face-face	-5.07793	-4.8576	-0.21308	-0.22033	-5.07068
cis-butterfly	-5.01498	-4.85118	-0.18278	-0.1638	-5.03396
trans-butterfly	-5.02175	-4.86847	-0.16093	-0.15328	-5.02939
zigzag-ladder	-4.98274	-4.81048	-0.21858	-0.17226	-5.02907
alternating-ladder	-4.67529	-4.51731	-0.17546	-0.15798	-4.69277
single-zigzag	-4.70333	-4.56213	-0.16554	-0.1412	-4.72767
square-columnar	-5.06613	-4.87964	-0.19651	-0.18649	-5.07615

TABLE S3. Table for P under 11.0 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=12.38 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-face-face	-5.0953	-4.87618	-0.21313	-0.21912	-5.08931
cis-butterfly	-5.00433	-4.85119	-0.18151	-0.15314	-5.0327
trans-butterfly	-5.01292	-4.86848	-0.15329	-0.14444	-5.02177
zigzag-ladder	-4.97052	-4.81049	-0.23108	-0.16003	-5.04157
alternating-ladder	-4.66539	-4.51731	-0.1617	-0.14808	-4.67901
single-zigzag	-4.69687	-4.56213	-0.16078	-0.13474	-4.72292
square-columnar	-5.05216	-4.87965	-0.1924	-0.17251	-5.07205

TABLE S4. Table for P under 12.38 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=8.25 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-edge-edge	-4.7823	-4.39036	-0.36506	-0.39195	-4.75541
tetramer-face-face	-4.77084	-4.40297	-0.3501	-0.36787	-4.75307
trans-butterfly	-4.89292	-4.44402	-0.37806	-0.4489	-4.82207
zigzag-ladder	-4.48775	-4.36402	-0.30629	-0.12374	-4.67031
alternating-ladder	-4.56638	-4.16873	-0.39175	-0.39765	-4.56048
single-zigzag	-4.7556	-4.12197	-0.46765	-0.63373	-4.58952
As8 chain	-4.47897	-4.09898	-0.47494	-0.37999	-4.57391

TABLE S5. Table for As under 8.25 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=9.63 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-edge-edge	-4.7283	-4.39243	-0.3119	-0.33587	-4.70433
tetramer-face-face	-4.83054	-4.40734	-0.30463	-0.4232	-4.71197
trans-butterfly	-4.74172	-4.4485	-0.30852	-0.29335	-4.75689
zigzag-ladder	-4.8143	-4.37649	-0.35189	-0.43781	-4.72839
alternating-ladder	-4.52915	-4.18819	-0.32681	-0.34096	-4.51501
single-zigzag	-4.31035	-4.12206	-0.31101	-0.18828	-4.43309
As8 chain	-4.76627	-4.35209	-0.33399	-0.41418	-4.68608

TABLE S6. Table for As under 9.63 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=11.0 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-edge-edge	-4.59672	-4.40282 -	0.19694	-0.20733	-4.58633
tetramer-face-face	-4.83132	-4.44037	-0.24269	-0.39096	-4.68305
trans-butterfly	-4.61324	-4.44819	-0.19639	-0.16483	-4.6448
zigzag-ladder	-4.68349	-4.37645	-0.24403	-0.30704	-4.62048
alternating-ladder	-4.39154	-4.18821	-0.21352	-0.20333	-4.40173
single-zigzag	-4.19255	-4.12211	-0.19577	-0.07038	-4.31795
As8 chain	-4.65432	-4.35083	-0.23418	-0.30341	-4.58509

TABLE S7. Table for As under 11.0 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=12.38 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-edge-edge	-4.59809	-4.39272	-0.19993	-0.20537	-4.59266
tetramer-face-face	-4.7182	-4.44286	-0.2564	-0.27526	-4.69935
trans-butterfly	-4.64842	-4.44859	-0.20203	-0.19983	-4.65061
zigzag-ladder	-4.60751	-4.37705	-0.27803	-0.23046	-4.65508
alternating-ladder	-4.3948	-4.18845	-0.23076	-0.20635	-4.41922
single-zigzag	-4.30326	-4.12216	-0.22034	-0.18109	-4.34251
As8 chain	-4.58453	-4.35217	-0.25409	-0.23236	-4.60626

TABLE S8. Table for As under 12.38 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=8.25 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-corner-face	-3.98506	-3.78336	-0.27962	-0.2017	-4.06298
tetramer-edge-edge	-4.06363	-3.7805	-0.42969	-0.28313	-4.2102
tetramer-face-face	-4.17665	-3.84038	-0.32732	-0.33627	-4.1677
zigzag-ladder	-3.72924	-3.78933	-0.04746	0.06009	-3.83679
trans-butterfly	-4.1835	-3.84734	-0.328	-0.33616	-4.17534
alternating-ladder	-3.96122	-3.67164	-0.33683	-0.28958	-4.00846
Sb8 chain	-3.75212	-3.67549	-0.37039	-0.07663	-4.04588

TABLE S9. Table for Sb under 8.25 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=9.63 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-corner-face	-4.16434	-3.79464	-0.38415	-0.3697	-4.17879
tetramer-edge-edge	-4.17161	-3.78768	-0.49526	-0.38393	-4.28294
tetramer-face-face	-4.18551	-3.8126	-0.41496	-0.37291	-4.22756
zigzag-ladder	-4.18662	-3.83538	-0.4342	-0.35124	-4.26958
trans-butterfly	-4.23849	-3.8571	-0.41523	-0.38139	-4.27233
alternating-ladder	-4.06194	-3.67616	-0.44757	-0.38578	-4.12373
Sb8 chain	-4.10658	-3.76937	-0.36167	-0.33721	-4.13105

TABLE S10. Table for Sb under 9.63 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=11.0 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-corner-face	-4.05575	-3.79468	-0.32307	-0.26107	-4.11776
tetramer-edge-edge	-4.04841	-3.78663	-0.3336	-0.26178	-4.12023
tetramer-face-face	-4.13171	-3.8477	-0.31207	-0.28401	-4.15977
zigzag-ladder	-4.12225	-3.83578	-0.33983	-0.28647	-4.1756
trans-butterfly	-4.11274	-3.85744	-0.28055	-0.2553	-4.13799
alternating-ladder	-3.93728	-3.67615	-0.30245	-0.26113	-3.97861
Sb8 chain	-4.0585	-3.77507	-0.31068	-0.28343	-4.08575

TABLE S11. Table for As under 11.0 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

$2R$=12.38 Å	E_b^{RDCP}	E_{inter}^{RDCP}	$E_c^{DFT}(segment)$	$E_c^{RDCP}(segment)$	E_b^{corr}
tetramer-corner-face	-4.04159	-3.79468	-0.30457	-0.24691	-4.09925
tetramer-edge-edge	-4.03325	-3.78663	-0.31365	-0.24662	-4.10027
tetramer-face-face	-4.14079	-3.85265	-0.30746	-0.28814	-4.16012
zigzag-ladder	-4.1149	-3.83583	-0.33133	-0.27907	-4.16717
trans-butterfly	-4.0965	-3.85743	-0.26354	-0.23907	-4.12097
alternating-ladder	-3.92181	-3.67616	-0.28419	-0.24565	-3.96035
Sb8 chain	-4.05307	-3.77505	-0.29878	-0.27802	-4.07383

TABLE S12. Table for Sb under 12.38 Å confinement (diameter). E_b^{RDCP} is the total binding energy under RDCP, including the inter-atomic interaction E_{inter}^{RDCP} calculated with DFT and confining interaction energy provided by RDCP. $E_c^{DFT}(segment)$ and $E_c^{RDCP}(segment)$ are the confining interaction energy of a corresponding segment calculated using DFT and RDCP, respectively. E_b^{corr} is the corrected total binding energy as defined in Eq. 1 of the main text.

	2R=8.25(Å)	2R=9.63(Å)	2R=11.0(Å)	2R=12.38(Å)
D(R)	-18.05	0.28	0.17	0.16
A(R)	1.59	4.41	5.76	7.27
B(R)	0.48	0.61	0.52	0.54
M(R)	12.28	-0.01	-0.04	-0.05

TABLE S13. D(R), A(R), B(R), and M(R) parameters for different carbon nanotubes. $2R$ is the diameter. The unit of D(R) is eV.