

Electronic Supplementary Information

Epitaxial Growth of Aligned Atomically Precise Chevron Graphene Nanoribbons on Cu(111)

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Section S1: Computational Details

The density functional theory (DFT) calculations performed used both VASP¹ and ADF²⁻⁴ for the periodic and molecular calculations, respectively. With both software packages, the PBE⁵ (Perdew-Burke-Ernzerhof) GGA functional was used in conjunction with the Grimme3 dispersion correction,⁶ coined PBE-D3. A plane wave basis set with an energy cutoff of 500 eV was used for all periodic calculations while a TZP⁷ (triple-zeta with polarization functions) basis set was used within the molecular calculations. The projector augmented wave (PAW) method^{8,9} for treating the core states was used as implemented within VASP, while the core electrons were frozen within the ADF calculations. In both sets of calculations, the Cu (4s/3d), C (2s/2p), and H (1s) electrons were treated explicitly. The *k*-space consisted of a 3 x 3 x 1 Monkhorst-Pack¹⁰ scheme for all calculations performed on the chevron-type GNR, and the molecular model used to represent it (C₄₂H₁₈) while adsorbed to the Cu(111) surface. For the gas-phase systems, we employed 3 x 3 x 1 *k*-point meshes if the results were compared with the surface-adsorbed systems, and 3 x 3 x 3 *k*-point meshes otherwise. All atoms were allowed to relax fully within the surface-adsorbate systems, except for the bottom two layers of the three layer Cu(111) surface, which were kept fixed using the experimental lattice constant of 3.62 Å. For the periodic calculations of the chevron-type GNR adsorbed to the Cu(111) surface, we employed either a 23.01 Å x (17.71 Å) x 30.00 Å unit cell or a (17.89 Å) x 22.14 Å x 30.00 Å unit cell, depending upon the growth direction of the GNR (see Figures S5 and S8). The number in parentheses denotes the periodic vector for the GNR lattice. Note that in both cases this unit cell vector is somewhat larger than the optimal lattice vector for the gas-phase GNR, being ~17.2 Å (see Section S3). However, it was prohibitively expensive to use larger unit cells that would potentially result in less substrate-induced strain within the adsorbate. Table S2 provides the destabilization of the gas-phase GNR for a variety of lattice vectors. The geometry optimizations were performed with a dipole correction applied to the *z*-axis. The charge density difference (CDD) plots were obtained by using the LCHARG tag within VASP.

References:

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Section S2: Binding Site Analysis of the C₄₂H₁₈ Molecular Model of the Chevron GNR

Binding Site	BE (eV)	ΔE (eV)	#C on T Site	C-Cu Dist. on T Site (Å)
H_{hcp}-30	-5.00	0	21	2.95-3.22
H _{fcc} -30	-4.97	0.03	21	2.95-3.21
Bridge-30	-4.95	0.05	21	3.01-3.32
Top-0	-4.86	0.14	16	2.99-3.19
Bridge-0	-4.86	0.14	16	3.04-3.22
H _{hcp} -0	-4.85	0.15	15	3.01-3.31
H _{fcc} -0	-4.85	0.15	15	2.99-3.30
Top-30	-4.54	0.46	0	-

Table S1: Binding site analysis of the C₄₂H₁₈ molecular model used for the chevron-type GNR on Cu(111), with the difference in energy relative to the most stable H_{hcp}-30 binding site (ΔE) and the binding energy (BE) displayed. The corrugation energy was calculated to be at least 0.46 eV. The number of carbon atoms on top sites (#C on T Site) and the range of C-Cu distances for the observed carbon atoms on the top sites (C-Cu Dist. on T Site) are given. The number of carbon atoms on top sites of the Cu(111) surface was determined by counting a carbon atom on a top site as a contribution of 1, and a C-C bond above a top site as a contribution of 1.

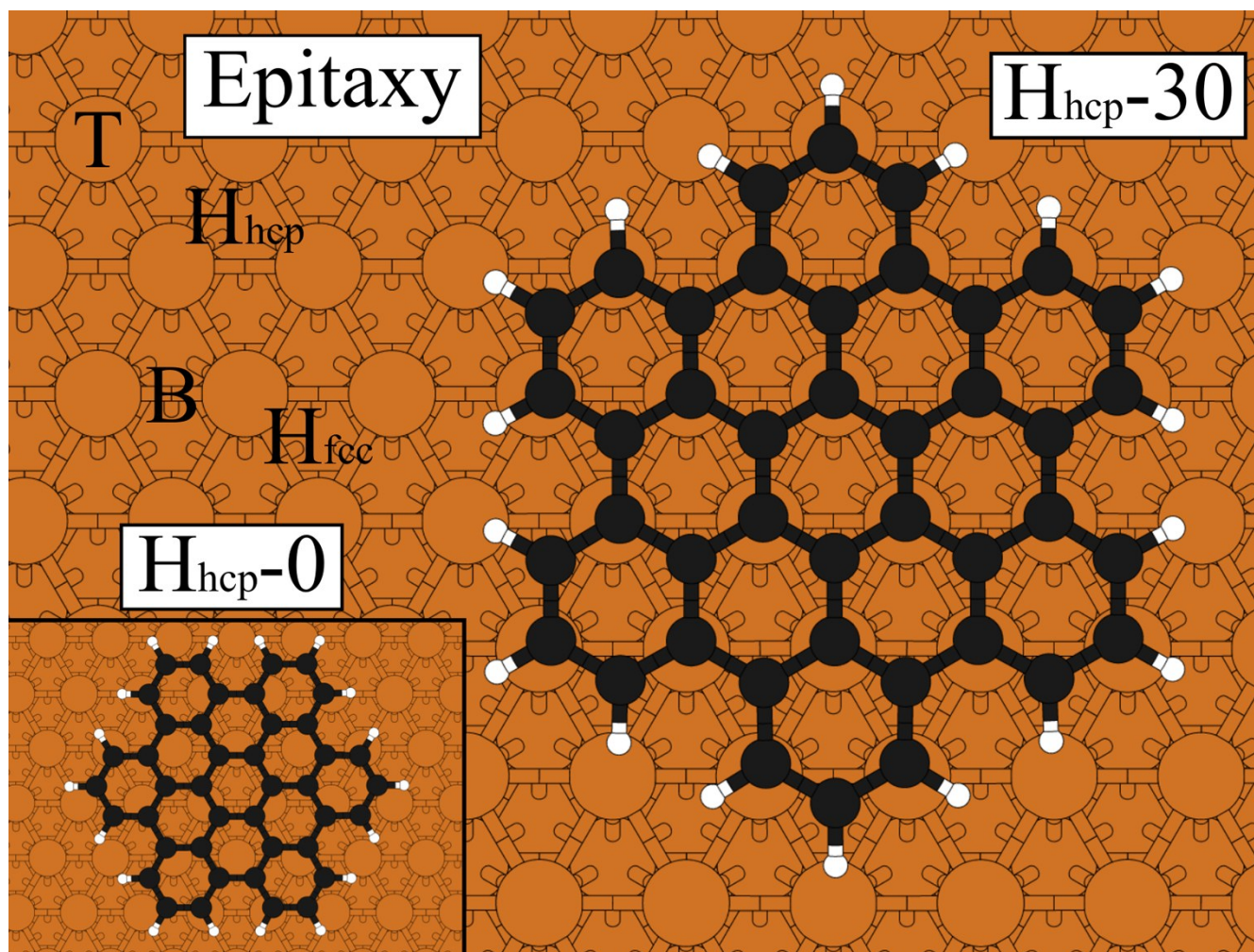


Figure S1: Eight high symmetry configurations for the adsorption of the $C_{42}H_{18}$ molecule (a model for the GNR) to the Cu(111) surface were considered. The central ring can be centered on top of a hollow hexagonal closed-packed (H_{hcp}) site, a hollow face centered cubic (H_{fcc}) site, a bridge (B) site, or a top (T) site. In addition, the ring can be rotated by 30° . Optimized geometries of $C_{42}H_{18}$ on the $H_{hcp}-30$ site and the $H_{hcp}-0$ site, resulting from a 30° rotation of the former, are shown in the main figure and the inset, respectively.

Section S3: Energy of the Chevron GNR as a Function of the Lattice Vector Employed

Length (Å)	ΔE (eV)
16.84	0.23
16.94	0.10
17.04	0.01
17.14	0.02
Gas-17.24	0
17.34	0.08
17.44	0.19
17.54	0.36
17.64	0.58
<112>/17.74	0.84
<110>/17.84	1.16

Table S2: The relative energy of the gas-phase GNR versus the lattice vector employed. The optimized lattice length was 17.24 Å. When the experimental Cu(111) lattice constant was employed to model the surface, the GNR lattice was stretched to 17.71 Å/17.89 Å so that it would fit on a periodic slab of the <112>/<110> surface. This lattice vector would lead to a destabilization of the gas-phase lattice by about 0.84/1.16 eV. In the calculations the z-direction was fixed for all of the atoms so that the system remained flat for each lattice vector chosen.

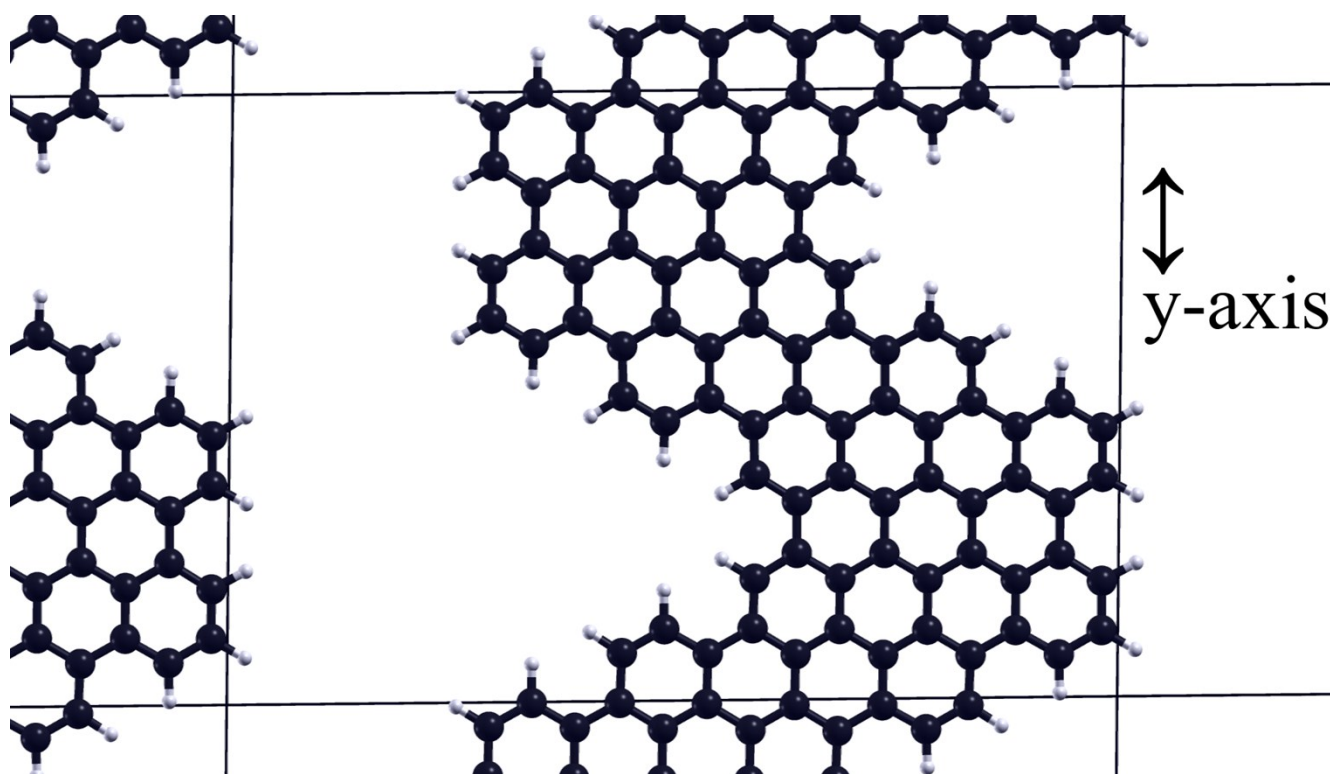


Figure S2: The chevron GNR in the gas-phase optimized with a 17.24 Å length in the y-direction.
Section S4: Comparison of the HOMO and LUMO of the C₄₂H₁₈ Molecule vs. Partial Charge Densities of the Chevron GNR

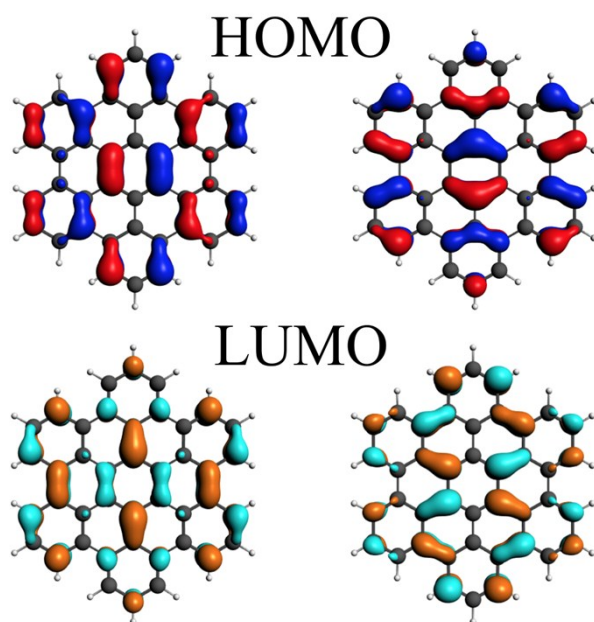


Figure S3: Isosurfaces of the doubly degenerate HOMOs (highest occupied molecular orbitals) and LUMOs (lowest unoccupied MOs) of the $C_{42}H_{18}$ molecule (isovalue = ± 0.03 au). Calculated using the ADF software package.

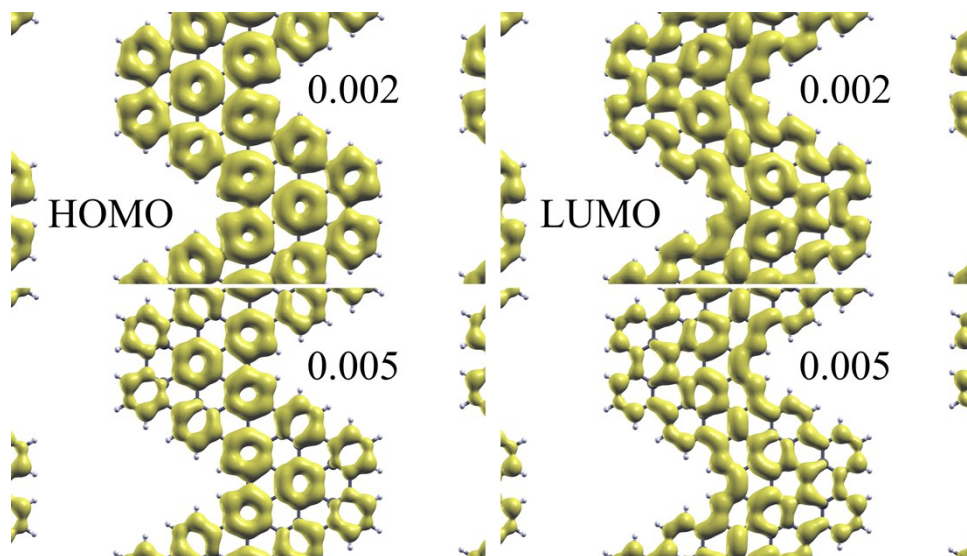


Figure S4: Partial charge densities (isovalue = $0.002 e/\text{\AA}^3$ or $0.005 e/\text{\AA}^3$) of the chevron GNR in the gas-phase. The range selected for the HOMOs and LUMOs were $(-0.25 - 0 \text{ eV})$ and $(+1.54 - +1.75 \text{ eV})$, respectively. Calculated using the VASP software package.

Visual inspection of Figure S3 and Figure S4 leads to the conclusion that the charge density of the GNR encompassing the energy range associated with the HOMOs/LUMOs resembles the frontier orbitals in the precursor $C_{42}H_{18}$ molecule.

Section S5: The Chevron GNR on Cu(111)

Binding Site	BE (eV)	ΔE (eV)	D(Surf-Ads) ($\text{\AA}$)
H_{hcp}-30	-8.79	0	2.98
H _{fcc} -30	-8.72	0.07	2.98
Bridge-30	-8.62	0.17	2.99
H _{hcp} -0	-8.63	0.16	3.01

Table S3: Binding site analysis of the chevron-type GNR on Cu(111), with the difference in binding energy relative to the most stable H_{hcp}-30 binding site (ΔE) and the binding energy (BE) displayed. The surface-adsorbate distance was calculated by averaging the carbon and hydrogen z-axis coordinates then subtracting an average of the copper z-axis coordinates within the top layer of the Cu(111) surface.

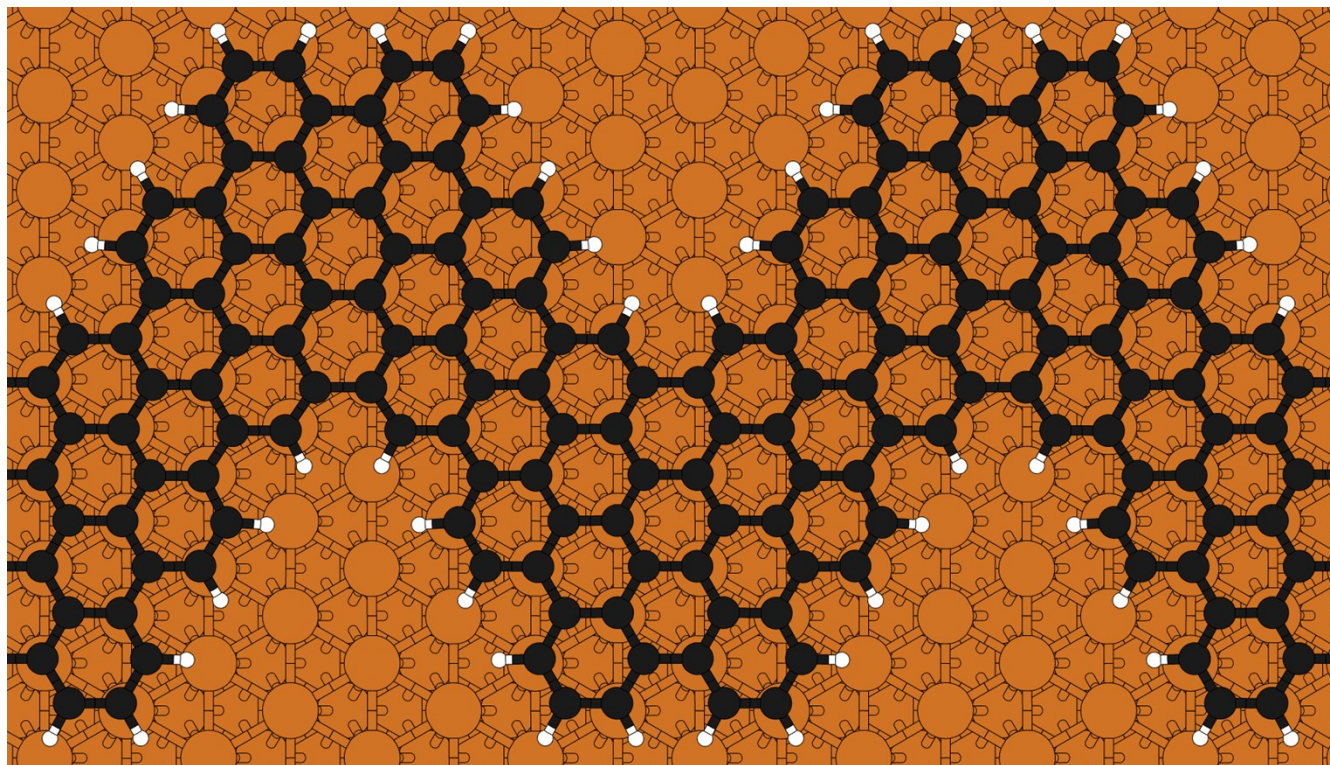


Figure S5: Optimized geometry of the chevron-type GNR on Cu(111) at the H_{hcp}-30 binding site. Within this model, each six membered carbon ring is centered on an H_{hcp} site and half of the carbon atoms lay on top of a Cu atom.

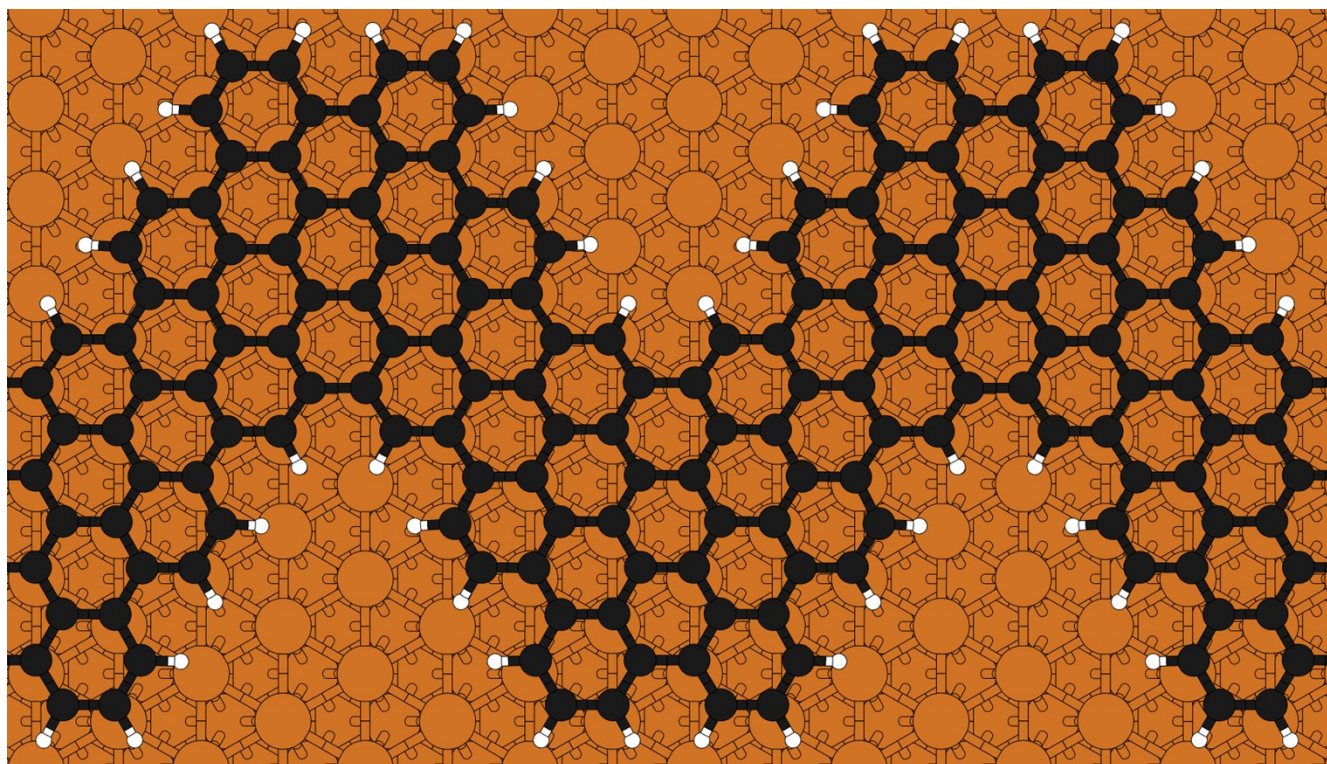


Figure S6: Optimized geometry of the chevron-type GNR on Cu(111) at the H_{fcc} -30 binding site. Within this model, each six membered carbon ring is centered on an H_{fcc} site and half of the carbon atoms lay on top of a Cu atom.

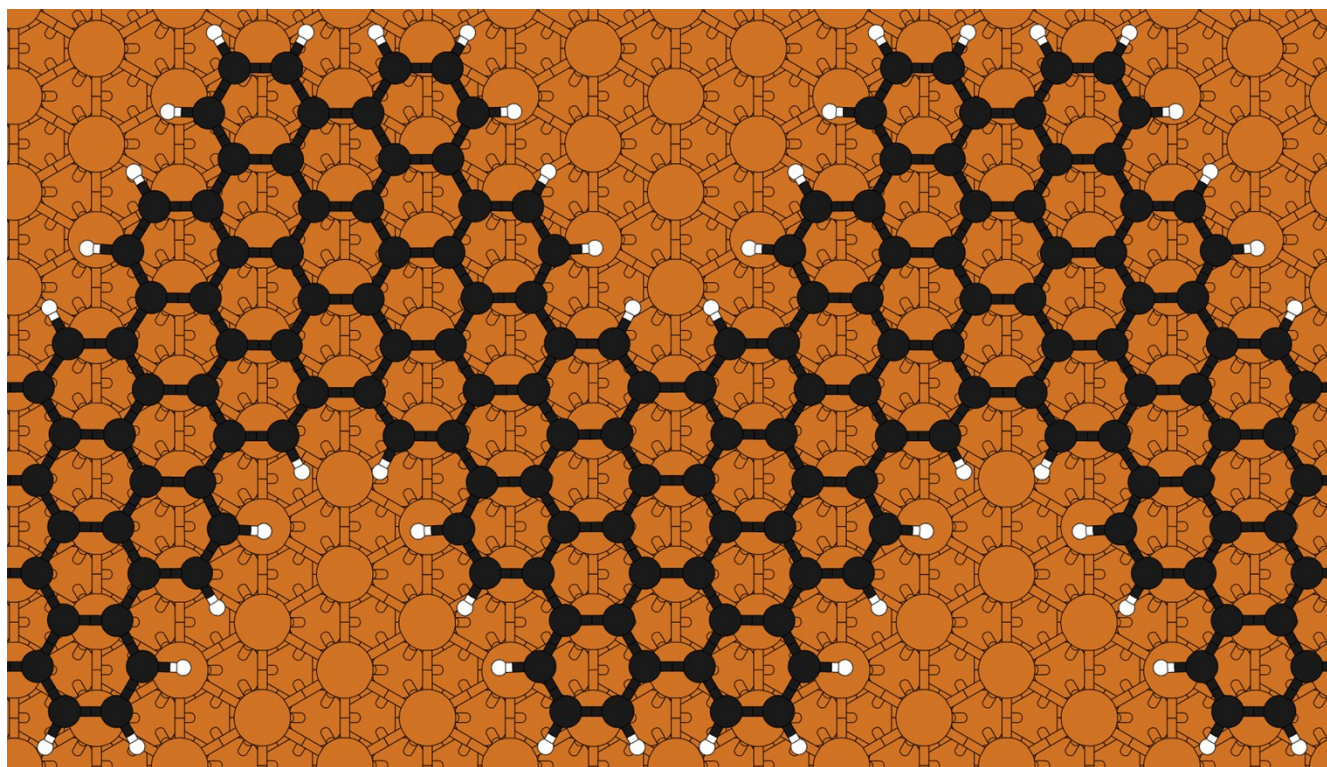


Figure S7: Optimized geometry of the chevron-type GNR on Cu(111) at the Bridge-30 binding site. Within this model, each six membered carbon ring is centered on a bridge site and 45% of the carbon atoms lay on top of a Cu atom, as estimated using the method explained in the caption to Table S1.

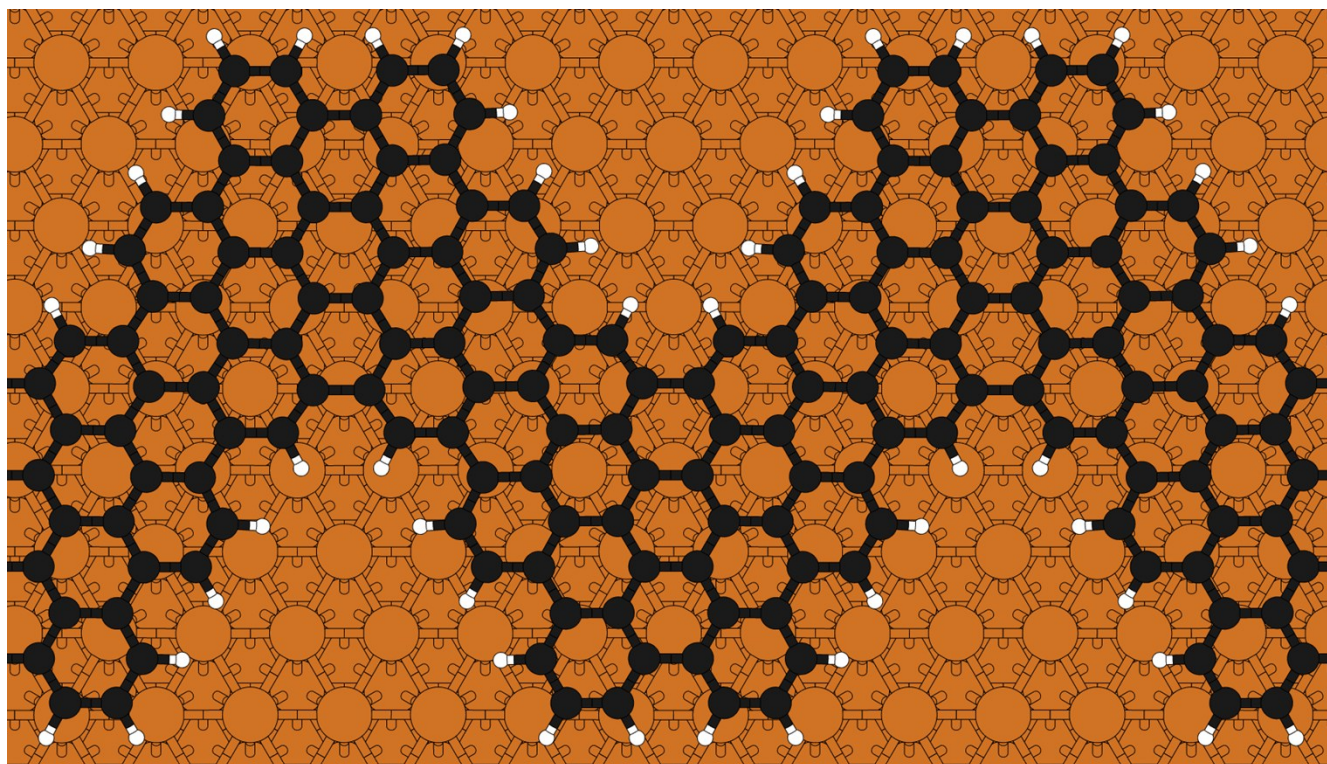


Figure S8: The chevron-type GNR on Cu(111) at the $H_{\text{hcp}}\text{-0}$ binding site. Within this model, the six membered carbon rings are centered on $H_{\text{hcp}}\text{-0}$, $H_{\text{fcc}}\text{-0}$, bridge, and top sites, with $\sim 36\%$ of the carbon atoms on top of a Cu atom, as calculated using the method explained in the caption to Table S1. The periodic lattice vector is $0.18 \text{ \AA}$ longer herein compared to Figures S5, S6, and S7. This model corresponds to growth along the $\langle 110 \rangle$ direction as opposed to the $\langle 112 \rangle$ direction. Since the lattice vector employed herein was larger than the growth in the $\langle 112 \rangle$ direction (see Table S2), the energetic destabilization of a gas phase GNR sheet in this geometry would be larger. The total binding energy for the $H_{\text{hcp}}\text{-0}$ site is $0.09 - 0.16 \text{ eV}$ smaller than the $H_{\text{fcc}}\text{-30}$ and $H_{\text{hcp}}\text{-30}$ sites (see Table S3).

Section S6: Charge Density Difference (CDD) Plots of the Chevron GNR on Cu(111)

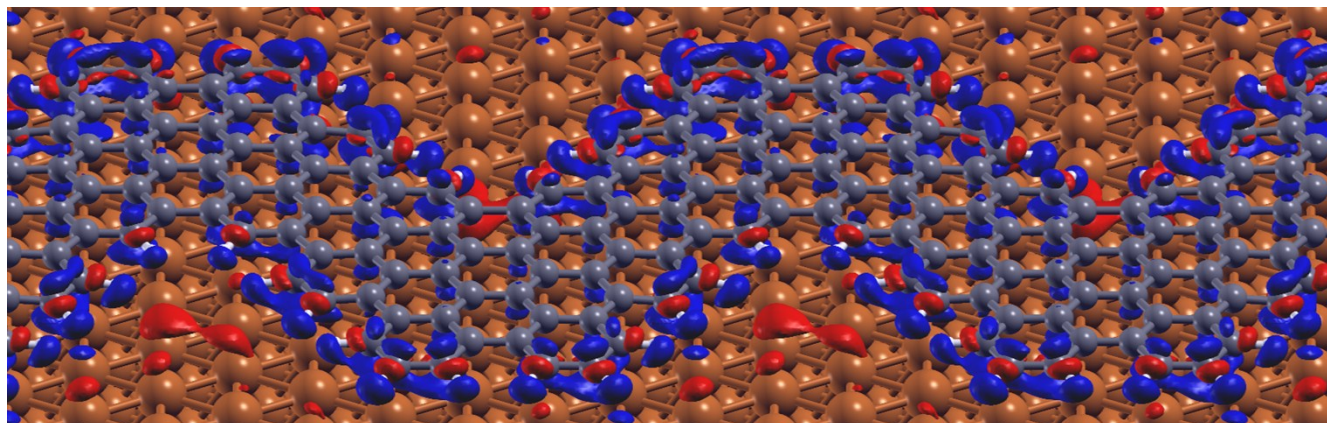


Figure S9: The CDD plot of the chevron-type GNR on Cu(111) in the $H_{\text{hcp}}\text{-}30$ site at an isovalue of $\pm 0.006 \text{ e}/\text{\AA}^3$, with the red/blue isosurfaces representing gain/loss of electronic charge density.

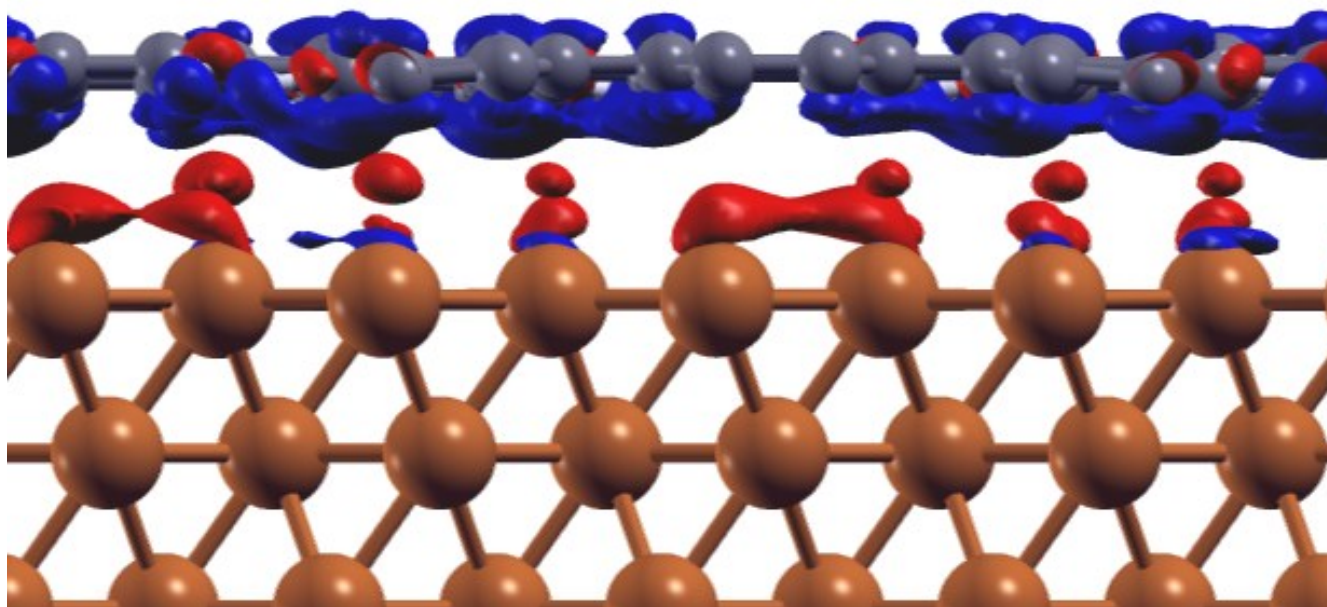


Figure S10: Same as Figure S9, but for a side view of the CDD. Note the red isosurfaces in the middle of the GNR and Cu(111) surface are indicative of weak chemisorption in the system.

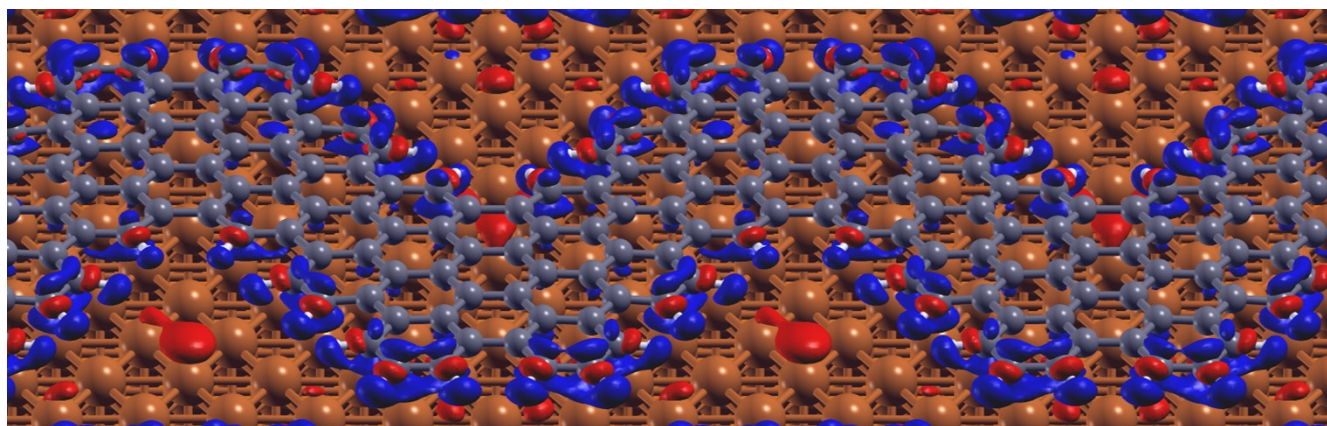


Figure S11: The CDD plot of the chevron-type GNR on Cu(111) in the $H_{\text{hcp}}-0$ site at an isovalue of $\pm 0.006 \text{ e}/\text{\AA}^3$, with the red/blue isosurfaces representing gain/loss of electronic charge density.

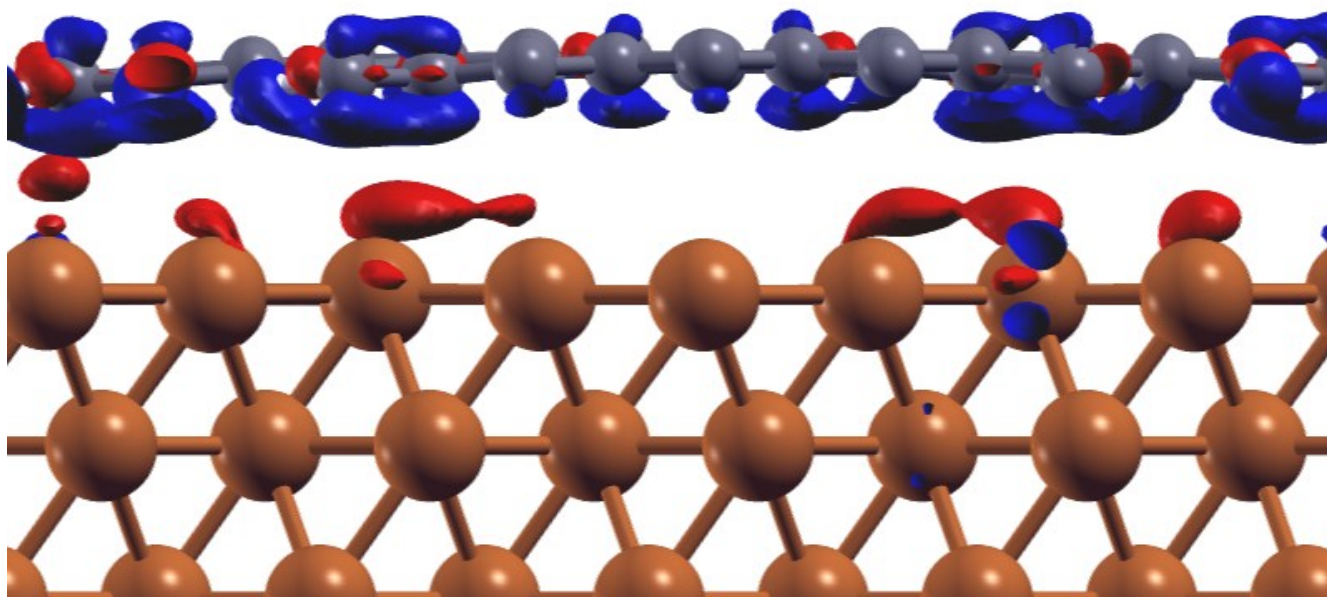


Figure S12: Same as Figure S11, but for a side view of the CDD. Note the red isosurface is smaller than in Figure S10, indicative of a weaker interaction.

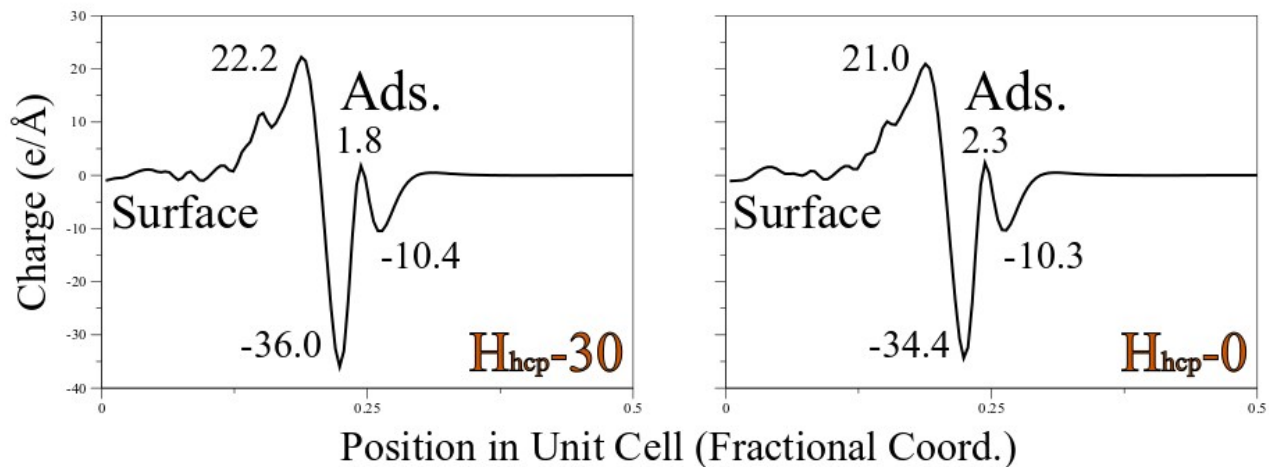


Figure S13: The plane-averaged CDD along the z -direction of the unit cell for the chevron-type GNR on Cu(111) in the (left) $H_{\text{hcp-30}}$ site ($\langle 112 \rangle$) and (right) $H_{\text{hcp-0}}$ site ($\langle 110 \rangle$). The charge gained above the surface is $22.2 \text{ e}/\text{\AA}$ / $21.0 \text{ e}/\text{\AA}$; the charge lost just below the adsorbate is $-36.0 \text{ e}/\text{\AA}$ / $-34.4 \text{ e}/\text{\AA}$; the charge gained in the adsorbate plane is $1.8 \text{ e}/\text{\AA}$ / $2.3 \text{ e}/\text{\AA}$; the charge lost just above the adsorbate is $-10.4 \text{ e}/\text{\AA}$ / $-10.3 \text{ e}/\text{\AA}$ for the $H_{\text{hcp-30}}/H_{\text{hcp-0}}$ sites. There is more charge transfer in the $H_{\text{hcp-30}}$ model.

Section S7: Fractional Coordinates of the Systems

Chevron-Type GNR on Cu(111) – Preferred H_{hcp}-30 Binding site and <112> Direction

Cu C H

1.0000000000000000		
23.0054400000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	17.709599999999982	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Cu C H

216 84 24

Direct

0.8888890000017398	0.7500000000000000	0.0000000000000000
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Chevron-Type GNR on Cu(111) – H_{hep}-0 Binding site and <110> Direction

Cu C H

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Cu C H

210 84 24

Direct

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0.5000279438886679	0.5666531146948515	0.0695666666666668
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0.1269757660310713	0.6835248837266228	0.2424477275961554
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0.6277262236219467	0.9002746510965430	0.2431171664114369
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0.2502917316491863	0.6272666057729999	0.2427748205797914
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0.7493641589823740	0.8446074521030644	0.2432654135098587
0.6681500743384251	0.8444562278999737	0.2433997824613355
0.3990349926146354	0.3054392533007916	0.2280245966675583
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0.2619685289777373	0.3049644151607121	0.2300560127633769
0.9004340018267042	0.4728094748051019	0.2303645456496078
0.5194974959835302	0.4728740632179086	0.2295858999002600
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0.8298923539698864	0.5644296016167131	0.2315332047022715
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0.7576477553693350	0.1668848094121094	0.2340954213037510
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Preferred Gas-Phase Periodic Lattice Vector to Chevron-Type GNR (17.24 Å)

C H

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0.1720963274229390 17.2396358251926642 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.5017708940888213

C H

84 24

Direct

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0.4889544022503713	0.7046382091049708	0.5000000000000000
0.4889842807136233	0.6209272887377466	0.5000000000000000
0.4891630492437002	0.4578167085237297	0.5000000000000000
0.4432264672252231	0.0787908556540131	0.5000000000000000
0.4413438616748451	0.9971034005032067	0.5000000000000000
0.4402621033913050	0.8305016222152446	0.5000000000000000
0.4399763491676083	0.7477711561204217	0.5000000000000000
0.4400818561681774	0.5812558861807346	0.5000000000000000
0.4418919787774982	0.4994814458704795	0.5000000000000000
0.3911703872985441	0.9571725961110005	0.5000000000000000
0.3909149371237959	0.8742682079798740	0.5000000000000000
0.3902323215827721	0.7076916514125529	0.5000000000000000
0.3899135662056636	0.6247163532565381	0.5000000000000000
0.3425483220308223	0.9985024568253351	0.5000000000000000
0.3414845025011246	0.8350675944777564	0.5000000000000000
0.3410998039284436	0.7503982681313417	0.5000000000000000
0.3408968223155497	0.5869677825420183	0.5000000000000000
0.2946309128836901	0.9599963786144556	0.5000000000000000
0.2940387665500594	0.8793858747002119	0.5000000000000000
0.2932582774008381	0.6290046725399776	0.5000000000000000
0.2932969144976809	0.7096270569791869	0.5000000000000000
0.0195883617700261	0.2184500710912332	0.5000000000000000
0.0193527749896489	0.3292355264835933	0.5000000000000000
0.0179687778396769	0.4716688820668153	0.5000000000000000
0.0192830208616357	0.0763349806653082	0.5000000000000000
0.9333720458431500	0.5447636802035731	0.5000000000000000
0.9352640271778725	0.0063927028923629	0.5000000000000000
0.8683936555600695	0.6002385052602648	0.5000000000000000
0.8697659137035316	0.9533950564563725	0.5000000000000000
0.7857923462958141	0.6719075245654267	0.5000000000000000
0.7873911686954216	0.8859224986571519	0.5000000000000000
0.7217358288424904	0.8334666094171794	0.5000000000000000
0.7207816666593203	0.7261084653932670	0.5000000000000000

0.5541220627793066	0.2309186822349076	0.5000000000000000
0.5533549338664940	0.3382594275856619	0.5000000000000000
0.4893606848862149	0.1803046281659277	0.5000000000000000
0.4874852469978066	0.3947357864296279	0.5000000000000000
0.4066777195895384	0.1135251635669263	0.5000000000000000
0.4052279721780891	0.4670720955159240	0.5000000000000000
0.3417645305128190	0.0616202596015967	0.5000000000000000
0.3396823118956505	0.5238997820889111	0.5000000000000000
0.2572878545835167	0.9932338132461851	0.5000000000000000
0.2557996609727269	0.8510816900022746	0.5000000000000000
0.2556797683687577	0.5985544059998418	0.5000000000000000
0.2553344428712379	0.7409043477731672	0.5000000000000000

Chevron-Type GNR in the Cu(111)-based Unit Cell (<112>)

C H

1.0000000000000000

23.0054400000000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.7095999999999982 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C H

84 24

Direct

0.3360577868207802	0.6878635534484677	0.2300846678045995
0.3361656440162183	0.6093954397945932	0.2294554658046668
0.3359564186142960	0.8520822296867948	0.2304655132439355
0.3358608445013300	0.9305168103828971	0.2299386007835393
0.3883677358958541	0.5705301036441629	0.2322447798819805
0.3880436217820140	0.7288993936217120	0.2338114949811077
0.3879954385268165	0.8110660762856502	0.2339349401338852
0.3879810955864070	0.9696209762090188	0.2323814223096560
0.4416388618771515	0.6089895808091567	0.2351973747825907
0.4419799782491433	0.6894022710792000	0.2364688236194831
0.4418752311314781	0.8508056896847195	0.2365364587683326
0.4413200561256844	0.9313077678584825	0.2352311433194553
0.4968030171343839	0.4888342630730623	0.2324518696023525
0.4961841537469906	0.5680120027204064	0.2362494997399036
0.4964201993012434	0.7297917766804498	0.2394000214298512
0.4963748971823828	0.8104660229840103	0.2393396272157685
0.4958096860159907	0.9723389604112781	0.2359875736023111
0.4964781261331990	0.0515679197582628	0.2322766249863192
0.5478827614415549	0.4484543004677162	0.2334141956635263
0.5498951733127287	0.6072032217189204	0.2396820391234442
0.5501531820034277	0.6890784585970310	0.2409456375223018
0.5500688495851337	0.8511821328992067	0.2407206264431529
0.5495359644013792	0.9330785862931458	0.2391641030839906
0.5475028726283162	0.0920731604223993	0.2329944671597100
0.6022967014886246	0.4839181431965942	0.2380949892500608
0.6031388221024410	0.5649673517520265	0.2403351217104163
0.6039347140538459	0.7292919653857904	0.2420077635154439
0.6038486738949237	0.8108840502883333	0.2419097122508090
0.6027201106148928	0.9754623507529695	0.2397128010233004
0.6019159941984479	0.0566327909853992	0.2374029122157454
0.6560603120327769	0.3582405383450832	0.2389860761917363
0.6556523493244132	0.4387485336106087	0.2396149096440916
0.6552634967653956	0.1018387417025032	0.2386906332854890
0.6557814800928833	0.1824544889302821	0.2383268866222688

0.6573895433087285	0.6053198612914659	0.2416626176584217
0.6578809976131634	0.6872008349213787	0.2419078383810320
0.6576984002896988	0.8530936638926226	0.2417638392675366
0.6569047444278031	0.9349685110031909	0.2412162574122096
0.7088656019759076	0.0616097600801084	0.2405466279636244
0.7064235926294865	0.2276080483963475	0.2400228683593177
0.7092109093216569	0.4788357596010918	0.2411762273269379
0.7065345579979569	0.3129531843846904	0.2402794274925251
0.7098113724725794	0.5615558915093252	0.2413277862033191
0.7120858576762643	0.7275762612501588	0.2410359503495946
0.7120262700117276	0.812835332453924	0.2410476317080514
0.7094002961487192	0.9788396360910633	0.2409466016464037
0.7616397538463094	0.4350763736355943	0.2417229463345148
0.7609339782036171	0.3531825956371206	0.2417111995430940
0.7608118599355012	0.1873367163506626	0.2414769057971396
0.7613914405909830	0.1054103381630728	0.2414768015447708
0.7632991460270163	0.6018602946352368	0.2400608184278529
0.7626959461126398	0.6823804708832978	0.2397381667956503
0.7625618519424482	0.8580627249077387	0.2399825074319016
0.7630262942240795	0.9386406523190263	0.2402324480066989
0.8159089815429595	0.4754873277451156	0.2409096337283537
0.8156624522357934	0.0649954781383746	0.2411323580357296
0.8148892390657585	0.3111091566847317	0.2420644034383961
0.8168245555969418	0.5567182040494397	0.2387651146699611
0.8148167138693693	0.2294815021218297	0.2420335624082052
0.8165548857848929	0.9836775305601657	0.2395100622475341
0.8686964275893616	0.1891818340493546	0.2417287381382535
0.8690801535696160	0.1072265260229290	0.2410305746361112
0.8711367953154314	0.9481030179584390	0.2363685132994458
0.8687879692239459	0.3514456005741894	0.2416983239230664
0.8692590030991877	0.4333853440609733	0.2408065892846253
0.8712682369256087	0.5923355322038927	0.2348842136353237
0.9222090179911718	0.9885699125222429	0.2362575306491170
0.9229570674150677	0.0679375830804824	0.2392181369544239
0.9225589124278470	0.2299400674111333	0.2411225904160072
0.9226029384463068	0.3106824885277343	0.2411130717024789
0.9223950077238580	0.5519937936131284	0.2349381738413737
0.9231287165530335	0.4727027803282237	0.2384271873915632
0.9776719041440197	0.1090059232873830	0.2390777512649376
0.9771722695863100	0.3510366167420217	0.2395267345791784
0.9770987976176317	0.1895473889492219	0.2397530620429767
0.9778080986850868	0.4316243606690370	0.2384035045931011
0.0312447893968964	0.0707615564870955	0.2374390590991161
0.0311493927099779	0.3113532612515417	0.2379434344376211
0.0311230546407158	0.2291863478415693	0.2380265233723552
0.0313872379577298	0.4698121045694427	0.2361962399989959
0.0834103661725305	0.1098311814841129	0.2352373897525775
0.0833079180098937	0.1882905983761478	0.2354161436108645
0.0833609769794137	0.3522048978480743	0.2353005573841494
0.0835931830565806	0.4306710674367375	0.2346056583448327
0.2945973151620715	0.7170790626197254	0.2276606835788683
0.2953095421555334	0.5784577559417372	0.2268317714814678
0.2945280175566721	0.8227243424183744	0.2282074693306674
0.2949058465867404	0.9612489424645017	0.2273586033636967
0.3871771722321758	0.5091497431302313	0.2321040291891101
0.3867371708788092	0.0309909021965252	0.2320254258312679

0.4564594621197469	0.4576503163439660	0.2283316874236326
0.4560455013207855	0.0826651642599508	0.2284369597415031
0.5454551352627037	0.3872915200682934	0.2301527021133796
0.5450329142459505	0.1532058383807464	0.2297031556865192
0.6143292689137746	0.3293438288963881	0.2372787044002075
0.6140939744842265	0.2114358746120686	0.2366446362036433
0.8044491109059464	0.7113006198751448	0.2385289928383072
0.8043311399259836	0.8291633967521050	0.2389243382497352
0.8738020536304175	0.8869042525206027	0.2335220309412979
0.8737801739654242	0.6534638947953655	0.2315705800352503
0.9627268266508761	0.9573187241171404	0.2333125035114652
0.9629051034617689	0.5831419314645775	0.2316246993893722
0.0325935103453526	0.0093646478022532	0.2374197666253088
0.0327055324714667	0.5311882182927927	0.2354742292366536
0.1244540090726241	0.0790554569252281	0.2332555458787577
0.1246602056127582	0.4612708233923255	0.2324712588939023
0.1248190407982538	0.3227671171446078	0.2337883276642130
0.1247845199038198	0.2175951690749558	0.2334937272929573

Chevron-Type GNR in the Cu(111)-based Unit Cell (<110>)

C H

1.0000000000000000		
17.8930000000000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	22.1370000000000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

C H

84 24

Direct

0.3696352389758038	0.3486381301353230	0.2300253310160967
0.0523370829429117	0.3483453795560589	0.2300665218678312
0.2920528828006974	0.3488049230298773	0.2303526373225657
0.1299161692500228	0.3487923280645350	0.2304098253949870
0.0133150058322576	0.4023969187089000	0.2323379639420228
0.9311934526375225	0.5150394523149723	0.2337855702784555
0.4892178668591077	0.5155110878285627	0.2328735292825771
0.4081655262467087	0.4028623693213165	0.2323329834045362
0.8905422108887234	0.5677748847284471	0.2347495730407086
0.5295868996920786	0.5682510523749482	0.2340651915905938
0.5474554971447172	0.1228796232680933	0.2346319710230295
0.4286219355653146	0.9561014897170119	0.2351326148160859
0.2514915148636679	0.4030358183461270	0.2332272062441300
0.1701784929626277	0.4030836648155785	0.2333208532077765
0.3885288099997789	0.9032221446339816	0.2357192557031362
0.8642770708749634	0.1244114915378598	0.2351275967807553
0.6249988251683747	0.1230015532402252	0.2352256545352193
0.7867443383041774	0.1236668779825358	0.2356157356578677
0.0508503773082036	0.4581485992964732	0.2351548316194542
0.3701436768475389	0.4584180852162738	0.2348767050184710
0.5091978717201067	0.0684567052640245	0.2360270072060212
0.9868566256979716	0.9579645154073353	0.2365864398614398
0.0279013279437268	0.9053649779750023	0.2371797254487450
0.0097692632945683	0.5147268618004670	0.2365334898033095
0.4106772431294641	0.5151002569486007	0.2359022507121501
0.1306065289554376	0.4590660127215361	0.2360104794095288
0.2904209664280112	0.4591702725420975	0.2356475837433077
0.9036992505812365	0.0704352758130552	0.2363219075848318

0.9249175127551662	0.6247201261115273	0.2382568722727398
0.7985683895585957	0.6798391108316103	0.2393568589373583
0.6206841526611412	0.6797004895452972	0.2395379155370186
0.6657253368027546	0.0688286464060170	0.2373791164943208
0.7469571670587916	0.0691225547788998	0.2374606745067701
0.4947643268641747	0.6248351990597559	0.2382202308248324
0.5475820065039355	0.0130782458368104	0.2377541338602573
0.5071445338796227	0.9564549649634566	0.2379884805749772
0.8788712925337405	0.6799495792021653	0.2393767484299498
0.8666772568712308	0.0144048831445267	0.2379698574711915
0.4237941140977809	0.8467263053812899	0.2391953435702200
0.2981082803742912	0.7920796663673167	0.2403932852515506
0.2501894403491248	0.5158111083196243	0.2382546458466583
0.1702027106950225	0.5158553346847955	0.2385374348227840
0.9081690995830527	0.9579595371687426	0.2385153664570478
0.1204644527009517	0.7927992809013843	0.2404623104700180
0.0482094095123502	0.5708427638950428	0.2393226362812705
-0.0060562610517385	0.8481395243365696	0.2399769903192609
0.5404581335248942	0.6797454263995160	0.2397355704069957
0.3718304228473020	0.5709621032173450	0.2389373700818547
0.6272294637199161	0.0124990382495222	0.2387195274592852
0.0056393552529022	0.6260726067222491	0.2400018362457814
0.7523134409462344	0.7318973612781364	0.2404847054944596
0.7869064900691705	0.0132991474307152	0.2387933926916813
0.6666507709268725	0.7317799422145234	0.2405817180058284
0.3782599702172945	0.7918156355611968	0.2404459909489914
0.0401523429703794	0.7929435414849737	0.2405522805017912
0.4140278293701933	0.6259874103795726	0.2400448244801148
0.1295093440497346	0.5716933090001923	0.2401046458373794
0.5464005445019265	0.9007027477324102	0.2400019064268135
0.2520194948624007	0.7401545496039738	0.2410811284414813
0.9182798567321288	0.7358407471049943	0.2407590103022482
0.2904756345670473	0.5717090455262795	0.2399422921726463
0.1665045720332382	0.7404999999866509	0.2410351114499609
0.8701354437049121	0.9015787203858480	0.2406155083560163
0.5044000999014517	0.8455868683930959	0.2404477189712728
0.0007844714170564	0.7369528667504399	0.2409618436985649
0.9131589466040413	0.8465726126010813	0.2410631943171719
0.5005306545775449	0.7352332042797313	0.2410427258855891
0.4180349384972697	0.7362102218428671	0.2412353219526049
0.8737144113157558	0.7898904277527381	0.2414683992259265
0.0452599564027066	0.6827671563148814	0.2410856582154616
0.6677313529674607	0.9559894308855846	0.2402412572034214
0.7920042798937423	0.7886570695102558	0.2413587685574139
0.7476788597080225	0.9563101172618601	0.2404610461606189
0.3737861233062522	0.6822711764294345	0.2413703728560700
0.6262751582034757	0.7882934102235359	0.2412903508559729
0.5445766013430936	0.7893086190331197	0.2413446423741758
0.1267937700490675	0.6837671039160252	0.2412623085992733
0.2921525688697721	0.6835258418568261	0.2414623255642769
0.6277021748780194	0.8999981947554433	0.2408613283358778
0.1691387540692006	0.6277977929583239	0.2411177286840867
0.2502581393998263	0.6276608348598998	0.2411412565761383
0.7887251428889431	0.9006215945320458	0.2411868839272928
0.7492820539528524	0.8444504750636221	0.2415680252859236
0.6681830072422743	0.8442383686665255	0.2413928074739026

0.4001559146804167	0.3060869755458694	0.2278276231124030
0.0221757318873746	0.3056224709594052	0.2278823125945787
0.2630016264535064	0.3057514056832897	0.2282701416243734
0.9007097037330432	0.4728245788635451	0.2301914348179768
0.5198548798237070	0.4734175858020784	0.2290806335456275
0.1592987184990390	0.3058692297678420	0.2284449796963040
0.8300066636123823	0.5646441869539471	0.2318417146161778
0.5901353617387246	0.5654948283108355	0.2312120563562768
0.3978459094492036	0.9982105475659833	0.2319878514598504
0.3279598430077090	0.9058557221355327	0.2330300938591981
0.5164754297305942	0.1652878976577743	0.2330900050581260
0.9525798363816341	0.4008029154110017	0.2319680125955355
0.4689080599942927	0.4016311531698855	0.2321461574294632
0.8940657186505566	0.1673628382669077	0.2336922196850531
0.0171764651015219	1.0004254504147789	0.2342007755326209
0.0885293701031431	0.9088480433754078	0.2352422738017485
0.7570516349764329	0.1665020575485897	0.2342872458192660
0.6536312389343726	0.1662908136638344	0.2341197163954857
0.4484572490658640	0.0694022145466589	0.2357714060479232
0.7707481424842890	0.6360598019622302	0.2384627575209762
0.6486176817469299	0.6359834806042927	0.2386096075352027
0.9644196399481492	0.0724648341264566	0.2361953748987344
0.2702594648605434	0.8358252414126924	0.2399773735900393
0.1484991104193616	0.8365171893490185	0.2401347776055737

Cu(111) Surface (<112>)

Cu

1.0000000000000000

23.0054400000000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.7095999999999982 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Cu

216

Direct

0.8888890000017398	0.7500000000000000	0.0000000000000000
0.9444450000000018	0.8750000000000000	0.0000000000000000
0.8888890000017398	0.5000000000000000	0.0000000000000000
0.9444450000000018	0.6250000000000000	0.0000000000000000
0.8888890000017398	0.2500000000000000	0.0000000000000000
0.9444450000000018	0.3750000000000000	0.0000000000000000
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[illegible]

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Cu

210

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0.8571508411110500	0.4000090346478729	0.0000000000000000
0.9285754205555250	0.4999774133803143	0.0000000000000000
0.8571508411110500	0.1999819307042543	0.0000000000000000
0.9285754205555250	0.2999954826760600	0.0000000000000000
0.8571508411110500	0.0000000000000000	0.0000000000000000
0.9285754205555250	0.1000135519718128	0.0000000000000000
0.7143016822221000	0.5999909653521271	0.0000000000000000
0.7857262616665750	0.7000045173239400	0.0000000000000000
0.7143016822221000	0.4000090346478729	0.0000000000000000
0.7857262616665750	0.4999774133803143	0.0000000000000000
0.7143016822221000	0.1999819307042543	0.0000000000000000
0.7857262616665750	0.2999954826760600	0.0000000000000000
0.7143016822221000	0.0000000000000000	0.0000000000000000
0.7857262616665750	0.1000135519718128	0.0000000000000000
0.5714525233331500	0.5999909653521271	0.0000000000000000
0.6428771027776250	0.7000045173239400	0.0000000000000000
0.5714525233331500	0.4000090346478729	0.0000000000000000
0.6428771027776250	0.4999774133803143	0.0000000000000000
0.5714525233331500	0.1999819307042543	0.0000000000000000
0.6428771027776250	0.2999954826760600	0.0000000000000000
0.5714525233331500	0.0000000000000000	0.0000000000000000
0.6428771027776250	0.1000135519718128	0.0000000000000000
0.4285474766668500	0.5999909653521271	0.0000000000000000
0.5000279438886679	0.7000045173239400	0.0000000000000000
0.4285474766668500	0.4000090346478729	0.0000000000000000
0.5000279438886679	0.4999774133803143	0.0000000000000000
0.4285474766668500	0.1999819307042543	0.0000000000000000
0.5000279438886679	0.2999954826760600	0.0000000000000000
0.4285474766668500	0.0000000000000000	0.0000000000000000
0.5000279438886679	0.1000135519718128	0.0000000000000000
0.2856983177779000	0.5999909653521271	0.0000000000000000
0.3571228972223750	0.7000045173239400	0.0000000000000000
0.2856983177779000	0.4000090346478729	0.0000000000000000
0.3571228972223750	0.4999774133803143	0.0000000000000000
0.2856983177779000	0.1999819307042543	0.0000000000000000
0.3571228972223750	0.2999954826760600	0.0000000000000000
0.2856983177779000	0.0000000000000000	0.0000000000000000
0.3571228972223750	0.1000135519718128	0.0000000000000000
0.1428491588889500	0.5999909653521271	0.0000000000000000
0.2142737383334250	0.7000045173239400	0.0000000000000000
0.1428491588889500	0.4000090346478729	0.0000000000000000
0.2142737383334250	0.4999774133803143	0.0000000000000000
0.1428491588889500	0.1999819307042543	0.0000000000000000
0.2142737383334250	0.2999954826760600	0.0000000000000000
0.1428491588889500	0.0000000000000000	0.0000000000000000
0.2142737383334250	0.1000135519718128	0.0000000000000000

0.0000000000000000	0.5999909653521271	0.0000000000000000
0.0714245794444750	0.7000045173239400	0.0000000000000000
0.0000000000000000	0.4000090346478729	0.0000000000000000
0.0714245794444750	0.4999774133803143	0.0000000000000000
0.0000000000000000	0.1999819307042543	0.0000000000000000
0.0714245794444750	0.2999954826760600	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0714245794444750	0.1000135519718128	0.0000000000000000
0.8571508411110500	0.8000180692957457	0.0000000000000000
0.9285754205555250	0.8999864480281872	0.0000000000000000
0.7143016822221000	0.8000180692957457	0.0000000000000000
0.7857262616665750	0.8999864480281872	0.0000000000000000
0.5714525233331500	0.8000180692957457	0.0000000000000000
0.6428771027776250	0.8999864480281872	0.0000000000000000
0.4285474766668500	0.8000180692957457	0.0000000000000000
0.5000279438886679	0.8999864480281872	0.0000000000000000
0.2856983177779000	0.8000180692957457	0.0000000000000000
0.3571228972223750	0.8999864480281872	0.0000000000000000
0.1428491588889500	0.8000180692957457	0.0000000000000000
0.2142737383334250	0.8999864480281872	0.0000000000000000
0.0000000000000000	0.8000180692957457	0.0000000000000000
0.0714245794444750	0.8999864480281872	0.0000000000000000

Molecular Model of the Chevron-Type GNR

C H

1.0000000000000000		
23.0054400000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	17.709599999999982	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

C H

42 18

Direct

0.5520038876035087	0.5826189470951566	0.2438704652510505
0.4983160362700624	0.6227642638958212	0.2439757905739845
0.4446887636526101	0.5822734361071992	0.2440977557767695
0.4448406016942719	0.5016185011405798	0.2439889706474927
0.4986438657710879	0.4615569255219149	0.2437489470633018
0.5522165829295049	0.5021049967088982	0.2437913946055057
0.4980003832493783	0.7044357556082138	0.2422111538212528
0.3902163353941356	0.6229861748813484	0.2426152832416322
0.3905939362867823	0.4606031275715465	0.2424499786173596
0.4988324907383716	0.3800346067307532	0.2420146820468179
0.6067377900693280	0.4617000911237992	0.2421348029575978
0.6062838422108316	0.6237308009526358	0.2421429172223833
0.6063610198453424	0.7043675070520220	0.2405691438493029
0.6595555156162051	0.7430545929263246	0.2378606319199489
0.7119252485991019	0.7040398718380962	0.2362940773884939
0.7122845845128146	0.6256121287895990	0.2377024671115664
0.6603090301319102	0.5841465234166999	0.2406404119329577
0.4443829806676795	0.7449760951656899	0.2407699667787705
0.4453245930021290	0.8241861698789666	0.2375035464673494
0.4974983634095639	0.8633979653442436	0.2356199958430370
0.5498493358778729	0.8244426106270808	0.2370989022200440
0.5513603965404267	0.7453296511137267	0.2403729342057885
0.3903726114000873	0.3800454880645709	0.2406649191176956
0.4454118949779865	0.3391418013758039	0.2403680674900567

0.5524724655153074	0.3396797285136766	0.2405054493039448
0.3367218563273783	0.5003693225882582	0.2411243645002506
0.3365397288687519	0.5827748956939878	0.2410556092051659
0.2843894573152147	0.6235016768611058	0.2378544923678921
0.2841157326031341	0.7019319227755991	0.2362552254854418
0.3361278541242625	0.7414847747229998	0.2379235067230693
0.3895980262960883	0.7035793949307136	0.2409867418971975
0.6605768252927081	0.5017519485561046	0.2405456904245956
0.7128070886992053	0.4608528084952451	0.2373887878331299
0.7128100926037031	0.3825023311365396	0.2356352582228750
0.6606597328039113	0.3431440462496878	0.2373810289410953
0.6072332707126635	0.3811507744459638	0.2405283216017641
0.5514748417455007	0.2605587611699846	0.2371445062062341
0.4992929368179623	0.2212101063491908	0.2355548371469798
0.4468929052311208	0.2600506017318323	0.2372130367636544
0.2847149540256462	0.4592197222853237	0.2381377466338768
0.2847853715888295	0.3808745423580444	0.2363499571436907
0.3370225178129874	0.3417673724672232	0.2377178362871165
0.2431685928102980	0.4884371355074822	0.2366028241385162
0.5918289393413452	0.2287054754373808	0.2352136466305539
0.6606304452529782	0.8043896133141585	0.2361725383360009
0.7528135408831671	0.7348850481408683	0.2334076998674003
0.7539216861363162	0.5966240071990395	0.2359211566756521
0.4974467955282337	0.9248050684674468	0.2325855220562094
0.5900220742786333	0.8567008698222351	0.2352327240710617
0.4049751639547360	0.8560463383676621	0.2358203280912332
0.2429776417046909	0.5940410581184161	0.2360157550883156
0.2430993792505690	0.7323581711221104	0.2331001291061111
0.3347511630537779	0.8027911654808495	0.2359335762239625
0.7542704296705339	0.4902731083540003	0.2356816340556496
0.7537735713382165	0.3518814554213455	0.2326154595702496
0.6619911406118110	0.2818282284897729	0.2357183897737092
0.4994768540879923	0.1598362357439430	0.2323378512839103
0.4067060651088381	0.2278104938655174	0.2354232122798059
0.2438620060806961	0.3501536490107645	0.2334412520815727
0.3359064454164437	0.2804452723565969	0.2357878147061386

Molecular Model of the Chevron-Type GNR on Cu(111) – Preferred H_{ncp}-30 Binding Site

Cu C H

1.0000000000000000

23.0054400000000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.7095999999999982 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Cu C H

216 42 18

Direct

0.0554947874083993	0.0413693646554663	0.1379366769794288
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0.0554641409097627	0.2911294300458849	0.1379833521865521
0.0000018531359061	0.4162165023375692	0.1379318555209039
0.0555114126152461	0.5413755788812509	0.1380195838489584
0.0000039701706243	0.6661397106594791	0.1379458609002242
0.0554960669428297	0.7910359744894180	0.1379839889386147
0.9999843582314512	0.9162507597033809	0.1379033718922926
0.1667745470520927	0.0413653377135503	0.1379618226405199
0.1112089378981338	0.1662361793822811	0.1379776204324230

0.1665771965498877 0.2911600201794258 0.1379526838769891
 0.1113613889354568 0.4163417800163671 0.1380818843065086
 0.1665603334808523 0.5411436754478061 0.1380924786433013
 0.1111698589522163 0.6661079646258941 0.1380562774033507
 0.1667675676788392 0.7911258722025494 0.1380263281152523
 0.1112998006479771 0.9163131285703727 0.1379237046970658
 0.2779707003652092 0.0415184373564941 0.1380973987129579
 0.2221441777625870 0.1660766281420578 0.1379583448212856
 0.2777949216499280 0.2909559090821716 0.1380808079100291
 0.2218667182897960 0.4163554643601657 0.1378257770963813
 0.2775516705736791 0.5412062884550863 0.1379234026098146
 0.2219501903104373 0.6663374377699611 0.1376689777113782
 0.2779012486613723 0.7912851494298252 0.1379396655774201
 0.2221460887778903 0.9163250694075984 0.1379675668960161
 0.3887394407104523 0.0413152871571683 0.1381385995912368
 0.3332052061502324 0.1659323046060166 0.1378554006395021
 0.3889488586240617 0.2909395582398346 0.1373965796401393
 0.3333051845609276 0.4164449290980627 0.1372444088533271
 0.3890981932022797 0.5411026774524075 0.1371631055019265
 0.3333187958915786 0.6666374780874307 0.1378610587545808
 0.3887307121437260 0.7914107495862055 0.1377329688965645
 0.3334540177695118 0.9162471915478179 0.1381100022246002
 0.4999665176773362 0.0408517301138147 0.1378339162021334
 0.4442413124014593 0.1658474498159279 0.1379784308074363
 0.5000040646594996 0.2915488670854884 0.1370874328658189
 0.4445824218906367 0.4162405496241917 0.1375173073207421
 0.5000256223237400 0.5412695241393024 0.1374882427195558
 0.4443930405731180 0.6660559066666920 0.1372252523365063
 0.5000638224566742 0.7914998015411641 0.1379382535005362
 0.4445863661798697 0.9166176106050443 0.1379698062766579
 0.6112290872528305 0.0412929610609396 0.1381311098673805
 0.5557457697257817 0.1658421121717808 0.1379934328868089
 0.6110622214302524 0.2909452700055724 0.1373739127680409
 0.5554569482166798 0.4162449916054527 0.1374900745405725
 0.6109787948445913 0.5410983528975493 0.1371488650983892
 0.5556765904149046 0.6660375463974759 0.1372152894171421
 0.6113343107717171 0.7913986624591800 0.1377194876314718
 0.5554291004900307 0.9166242119056633 0.1379744152123195
 0.7219874556437347 0.0415319806281431 0.1380999310190205
 0.6667652767175341 0.1659069121755152 0.1378459883378582
 0.7222053045710339 0.2909077063959558 0.1380799369239227
 0.6667507441365359 0.4164387902551354 0.1372165810936963
 0.7225184276082004 0.5412011394799592 0.1378970693318777
 0.6667894702399977 0.6666470175692254 0.1378487178905061
 0.7221370843386481 0.7913014891500794 0.1379342041369895
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 0.7778278617242478 0.1660701293039395 0.1379657464280299
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 0.7781654290935052 0.4163345542138472 0.1378147989081882
 0.8334576220239569 0.5411337112007573 0.1380964099498385
 0.7781015980907426 0.6663190252758255 0.1376661046126060
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 0.8887535879193322 0.1662298277057630 0.1379815499154518

0.9445249271445917	0.2911247776305927	0.1379877993107144
0.8886465410558557	0.4163238108295246	0.1380840634742810
0.9444984569896988	0.5413756060599297	0.1380200969613199
0.8888445508050751	0.6661072896233762	0.1380579509150692
0.9445080282854903	0.7910407135722863	0.1379846175049622
0.8886805340643846	0.9163162386325752	0.1379261428860161
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0.0000000000000000	0.3333340000000007	0.0695699999999988
0.0555559999982620	0.4583340000000007	0.0695699999999988
0.0000000000000000	0.5833340000000007	0.0695699999999988
0.0555559999982620	0.7083340000000007	0.0695699999999988
0.0000000000000000	0.8333340000000007	0.0695699999999988
0.0555559999982620	0.9583340000000007	0.0695699999999988
0.1111109999982602	0.0833340000000007	0.0695699999999988
0.1666670000008708	0.2083340000000007	0.0695699999999988
0.1111109999982602	0.3333340000000007	0.0695699999999988
0.1666670000008708	0.4583340000000007	0.0695699999999988
0.1111109999982602	0.5833340000000007	0.0695699999999988
0.1666670000008708	0.7083340000000007	0.0695699999999988
0.1111109999982602	0.8333340000000007	0.0695699999999988
0.1666670000008708	0.9583340000000007	0.0695699999999988
0.2222220000008690	0.0833340000000007	0.0695699999999988
0.2777779999991310	0.2083340000000007	0.0695699999999988
0.2222220000008690	0.3333340000000007	0.0695699999999988
0.2777779999991310	0.4583340000000007	0.0695699999999988
0.2222220000008690	0.5833340000000007	0.0695699999999988
0.2777779999991310	0.7083340000000007	0.0695699999999988
0.2222220000008690	0.8333340000000007	0.0695699999999988
0.2777779999991310	0.9583340000000007	0.0695699999999988
0.3333340000017415	0.0833340000000007	0.0695699999999988
0.3888890000017398	0.2083340000000007	0.0695699999999988
0.3333340000017415	0.3333340000000007	0.0695699999999988
0.3888890000017398	0.4583340000000007	0.0695699999999988
0.3333340000017415	0.5833340000000007	0.0695699999999988
0.3888890000017398	0.7083340000000007	0.0695699999999988
0.3333340000017415	0.8333340000000007	0.0695699999999988
0.3888890000017398	0.9583340000000007	0.0695699999999988
0.4444450000000018	0.0833340000000007	0.0695699999999988
0.5000000000000000	0.2083340000000007	0.0695699999999988
0.4444450000000018	0.3333340000000007	0.0695699999999988
0.5000000000000000	0.4583340000000007	0.0695699999999988
0.4444450000000018	0.5833340000000007	0.0695699999999988
0.5000000000000000	0.7083340000000007	0.0695699999999988
0.4444450000000018	0.8333340000000007	0.0695699999999988
0.5000000000000000	0.9583340000000007	0.0695699999999988
0.5555559999982620	0.0833340000000007	0.0695699999999988
0.6111109999982602	0.2083340000000007	0.0695699999999988
0.5555559999982620	0.3333340000000007	0.0695699999999988
0.6111109999982602	0.4583340000000007	0.0695699999999988
0.5555559999982620	0.5833340000000007	0.0695699999999988
0.6111109999982602	0.7083340000000007	0.0695699999999988
0.5555559999982620	0.8333340000000007	0.0695699999999988
0.6111109999982602	0.9583340000000007	0.0695699999999988
0.6666670000008708	0.0833340000000007	0.0695699999999988
0.7222229999991328	0.2083340000000007	0.0695699999999988

0.6666670000008708	0.3333340000000007	0.0695699999999988
0.7222229999991328	0.4583340000000007	0.0695699999999988
0.6666670000008708	0.5833340000000007	0.0695699999999988
0.7222229999991328	0.7083340000000007	0.0695699999999988
0.6666670000008708	0.8333340000000007	0.0695699999999988
0.7222229999991328	0.9583340000000007	0.0695699999999988
0.7777779999991310	0.0833340000000007	0.0695699999999988
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0.7777779999991310	0.3333340000000007	0.0695699999999988
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0.7777779999991310	0.5833340000000007	0.0695699999999988
0.8333340000017415	0.7083340000000007	0.0695699999999988
0.7777779999991310	0.8333340000000007	0.0695699999999988
0.8333340000017415	0.9583340000000007	0.0695699999999988
0.8888890000017398	0.0833340000000007	0.0695699999999988
0.9444450000000018	0.2083340000000007	0.0695699999999988
0.8888890000017398	0.3333340000000007	0.0695699999999988
0.9444450000000018	0.4583340000000007	0.0695699999999988
0.8888890000017398	0.5833340000000007	0.0695699999999988
0.9444450000000018	0.7083340000000007	0.0695699999999988
0.8888890000017398	0.8333340000000007	0.0695699999999988
0.9444450000000018	0.9583340000000007	0.0695699999999988
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0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0555559999982620	0.3750000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0000000000000000
0.0555559999982620	0.6250000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0555559999982620	0.8750000000000000	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.1666670000008708	0.1250000000000000	0.0000000000000000
0.1111109999982602	0.0000000000000000	0.0000000000000000
0.1666670000008708	0.3750000000000000	0.0000000000000000
0.1111109999982602	0.2500000000000000	0.0000000000000000
0.1666670000008708	0.6250000000000000	0.0000000000000000
0.1111109999982602	0.5000000000000000	0.0000000000000000
0.1666670000008708	0.8750000000000000	0.0000000000000000
0.1111109999982602	0.7500000000000000	0.0000000000000000
0.2777779999991310	0.1250000000000000	0.0000000000000000
0.2222220000008690	0.0000000000000000	0.0000000000000000
0.2777779999991310	0.3750000000000000	0.0000000000000000
0.2222220000008690	0.2500000000000000	0.0000000000000000
0.2777779999991310	0.6250000000000000	0.0000000000000000
0.2222220000008690	0.5000000000000000	0.0000000000000000
0.2777779999991310	0.8750000000000000	0.0000000000000000
0.2222220000008690	0.7500000000000000	0.0000000000000000
0.3888890000017398	0.1250000000000000	0.0000000000000000
0.3333329999991292	0.0000000000000000	0.0000000000000000
0.3888890000017398	0.3750000000000000	0.0000000000000000
0.3333329999991292	0.2500000000000000	0.0000000000000000
0.3888890000017398	0.6250000000000000	0.0000000000000000
0.3333329999991292	0.5000000000000000	0.0000000000000000
0.3888890000017398	0.8750000000000000	0.0000000000000000
0.3333329999991292	0.7500000000000000	0.0000000000000000
0.5000000000000000	0.1250000000000000	0.0000000000000000
0.4444440000017380	0.0000000000000000	0.0000000000000000

0.5000000000000000	0.3750000000000000	0.0000000000000000
0.4444440000017380	0.2500000000000000	0.0000000000000000
0.5000000000000000	0.6250000000000000	0.0000000000000000
0.4444440000017380	0.5000000000000000	0.0000000000000000
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