Supporting Informations

Designing all graphdiyne materials as graphene derivatives: topologically driven modulation of electronic properties

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[2]*Dipartimento di Chimica, Università degli Studi di Milano, 20133 Milano, Italy*
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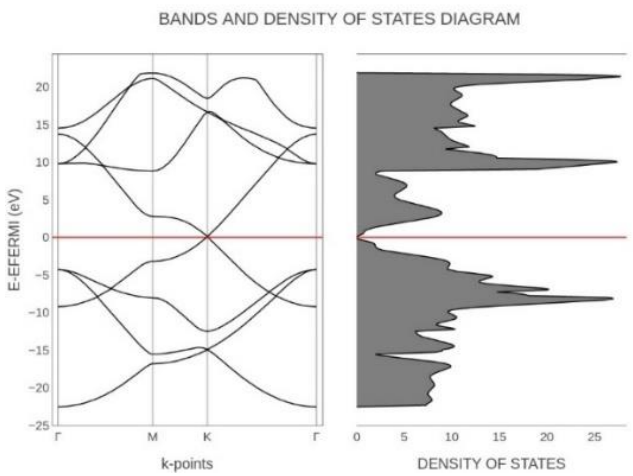
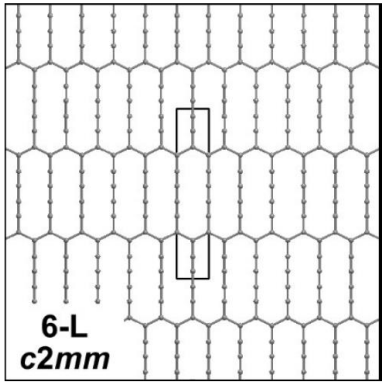
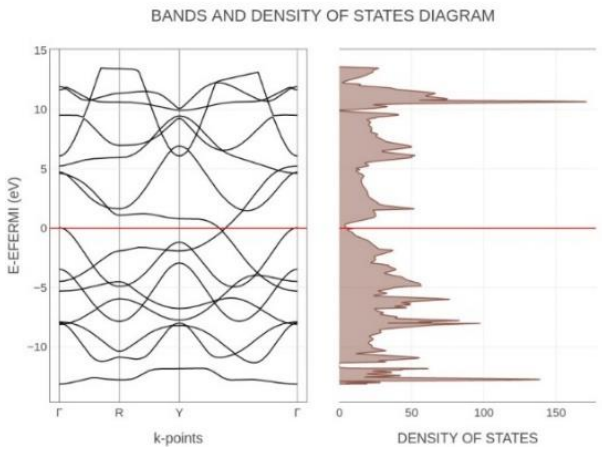
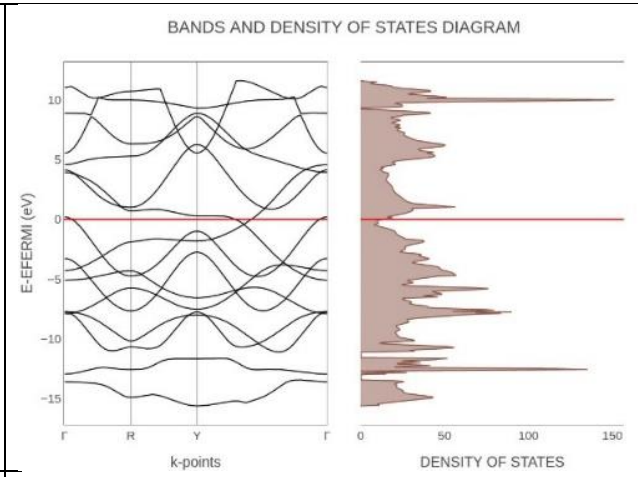
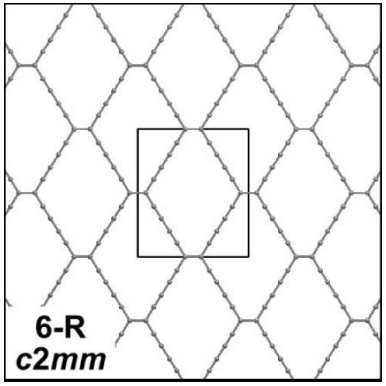
Table S1: *Computed band structures and density of states (DOS), with a sketch of the structure for each of the analysed 2D crystal, are reported. For some specific cases, a comparison between band structures and DOS calculated with PBE0 and HSE06 exchange-correlation density functionals is reported.*

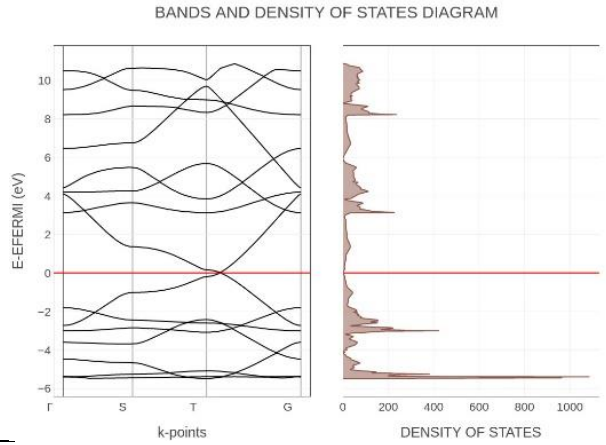
Names	Band Structure + DOS (PBE0)	Band Structure + DOS (HSE06)
Graphene		

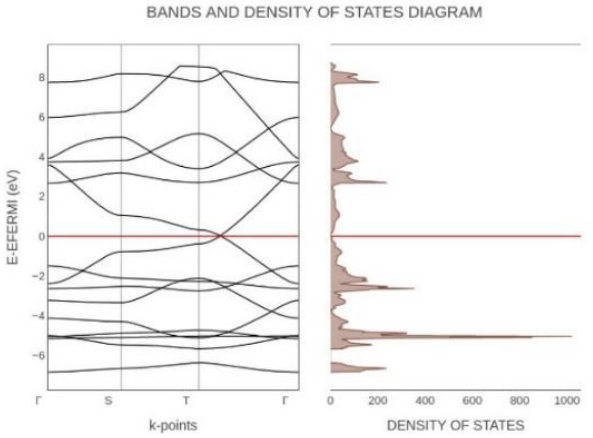

6-L
c2mm

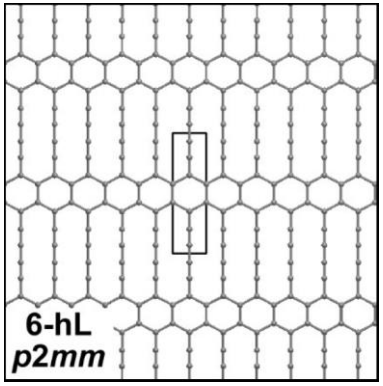

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ R Y Γ
k-points
0 50 100 150
DENSITY OF STATES

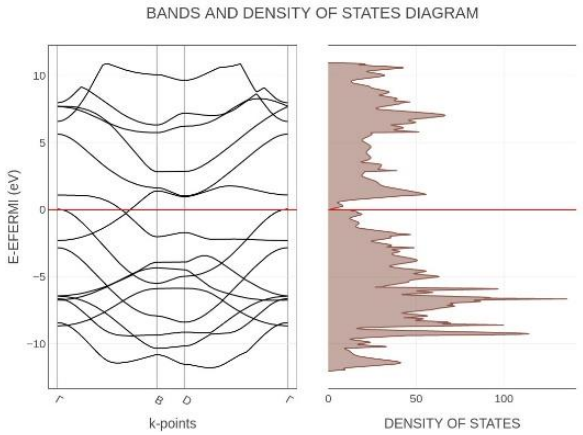

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ R Y Γ
k-points
0 50 100 150
DENSITY OF STATES

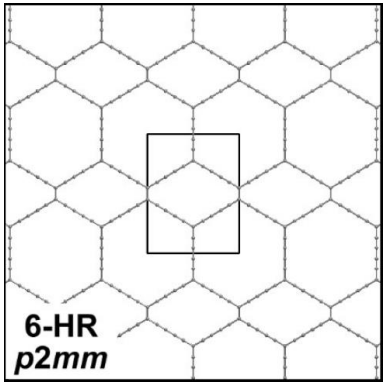

6-R
c2mm

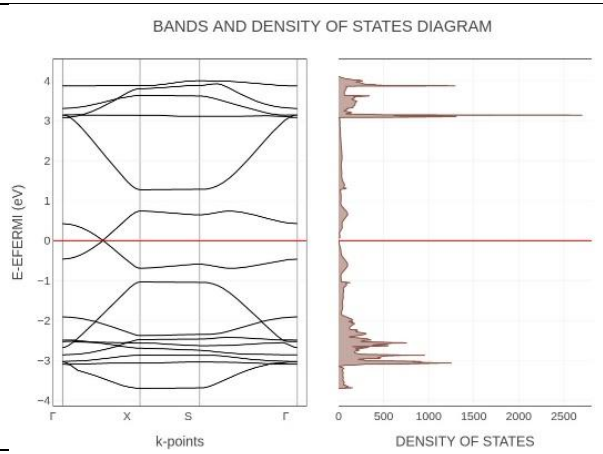

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ S T G
k-points
0 200 400 600 800 1000
DENSITY OF STATES

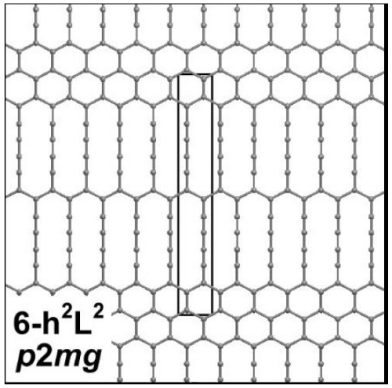

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ S T Γ
k-points
0 200 400 600 800 1000
DENSITY OF STATES

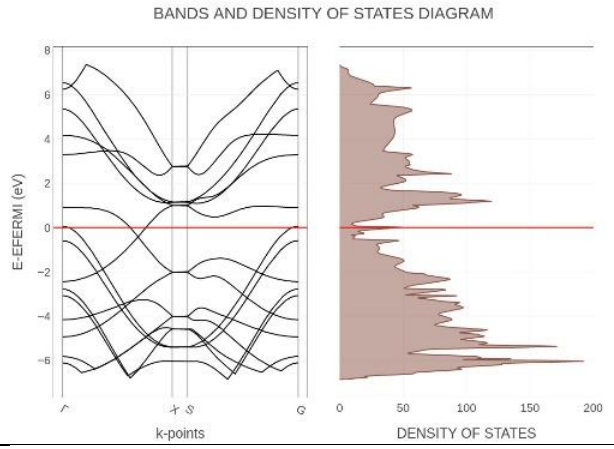

6-hL
p2mm

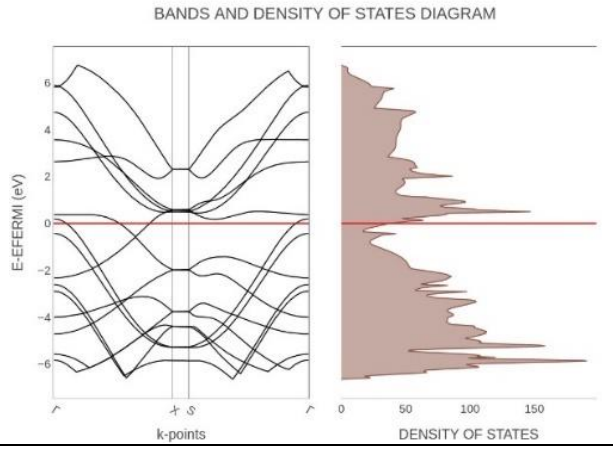

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ B D Γ
k-points
0 50 100
DENSITY OF STATES

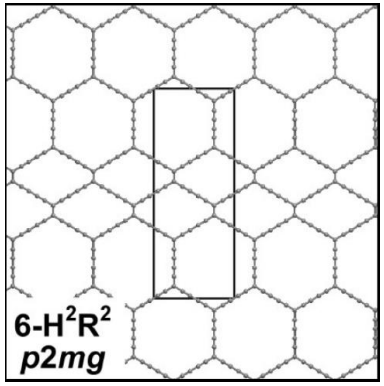

6-HR
p2mm

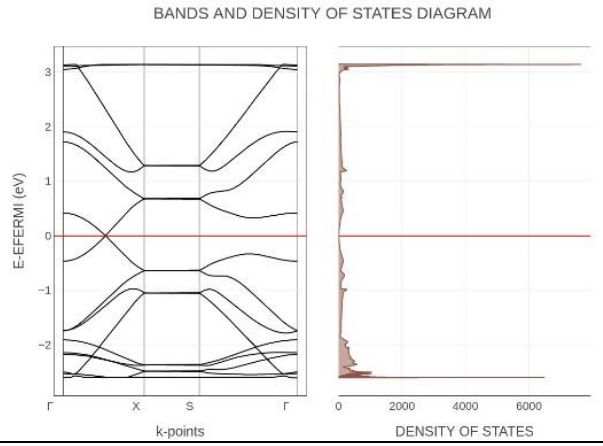

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES

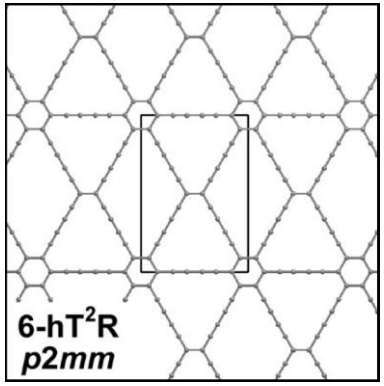

6-h²L²
p2mg

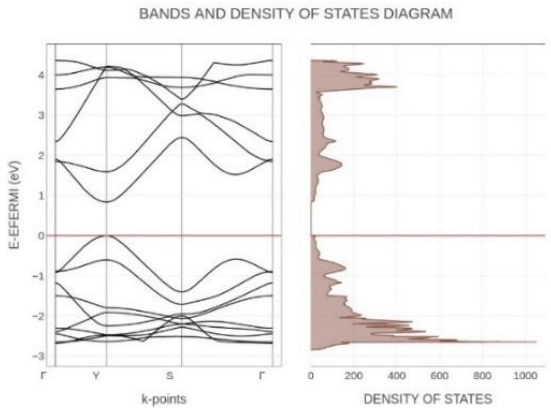

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES

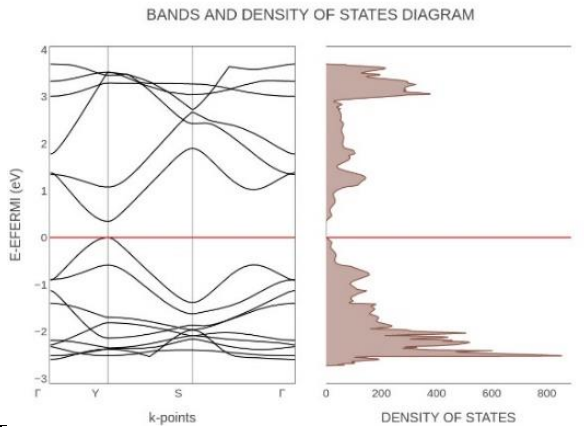

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES

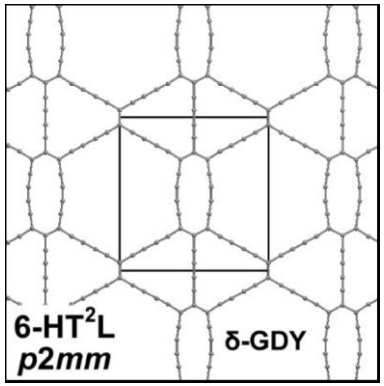

6-H²R²
p2mg

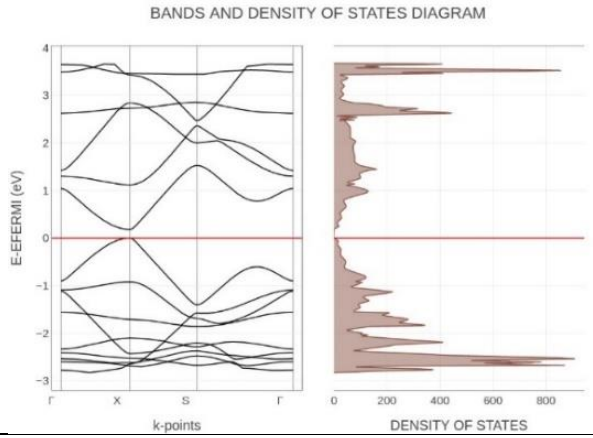

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES

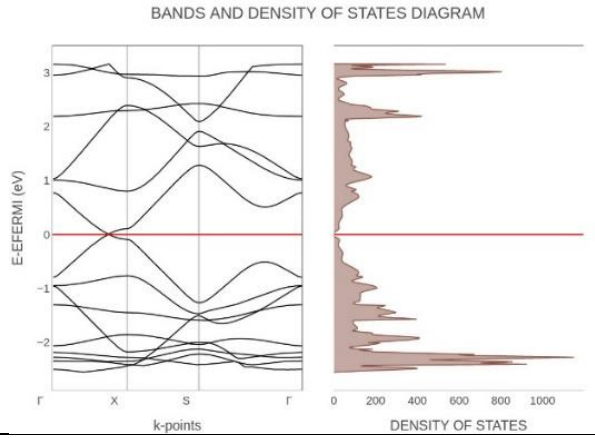

6-hT²R
p2mm

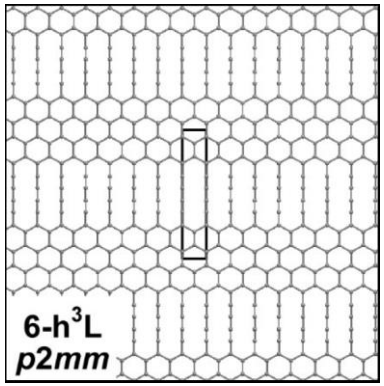

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES

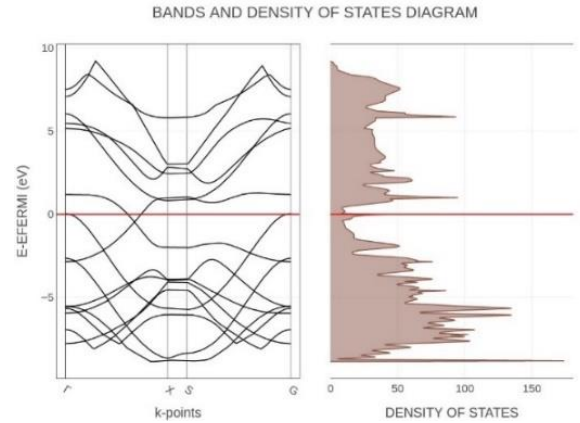

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES


6-HT²L
p2mm
δ-GDY


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
k-points
DENSITY OF STATES


6-h³L
p2mm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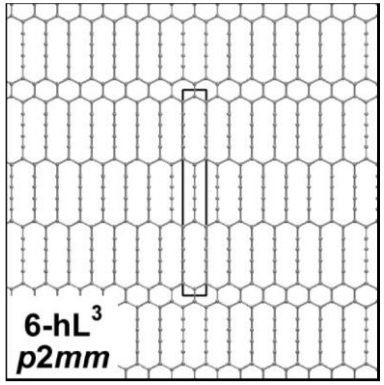
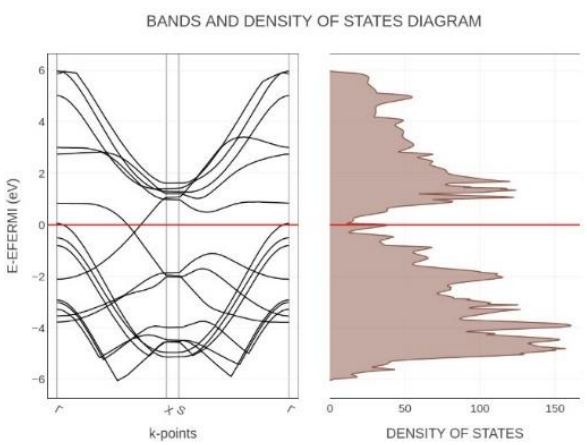
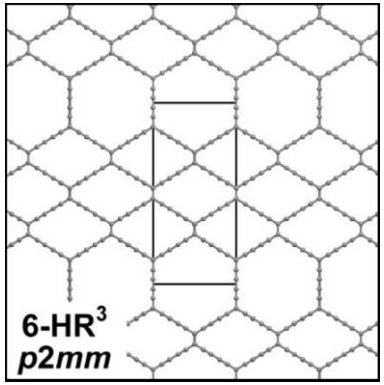
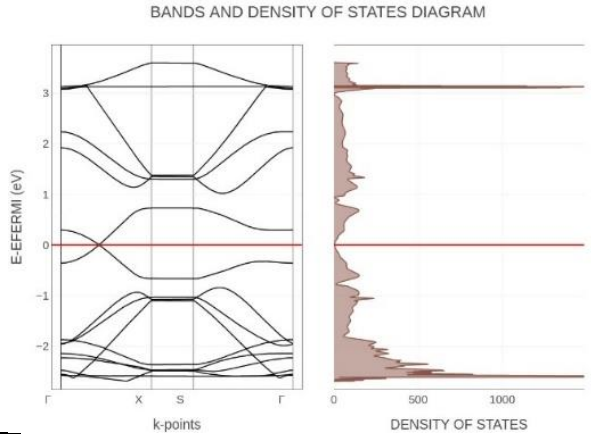
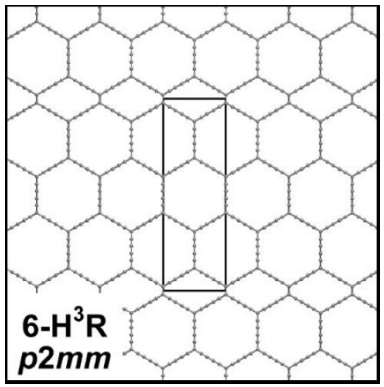
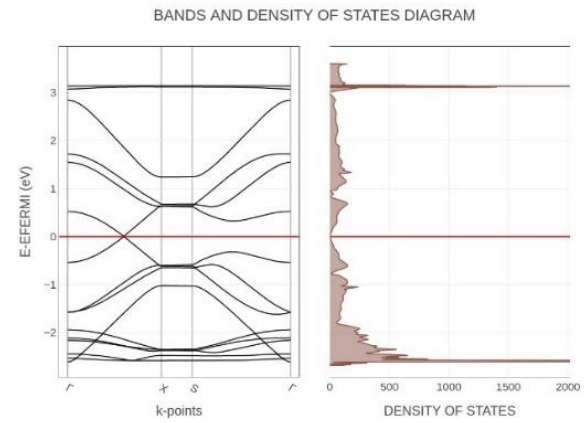
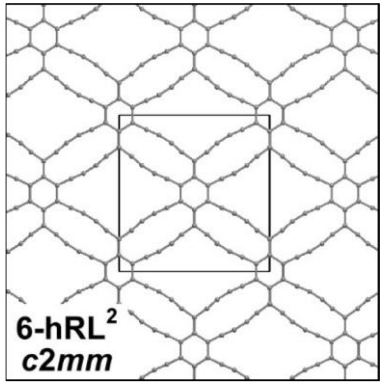
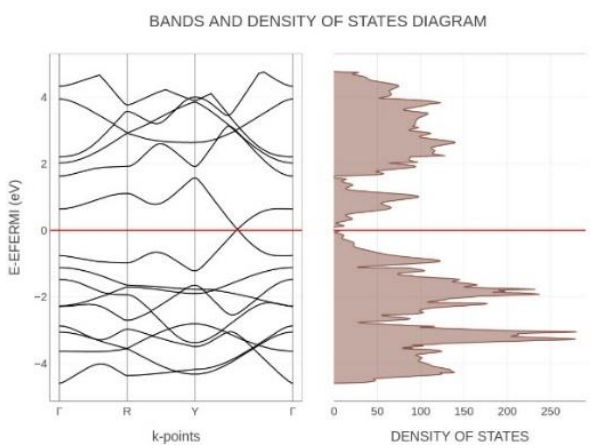
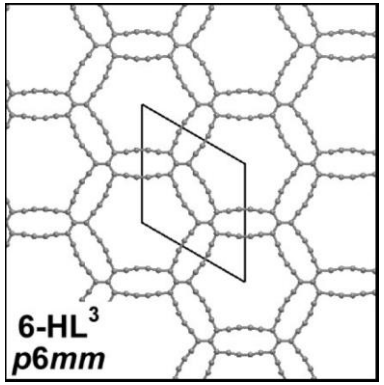
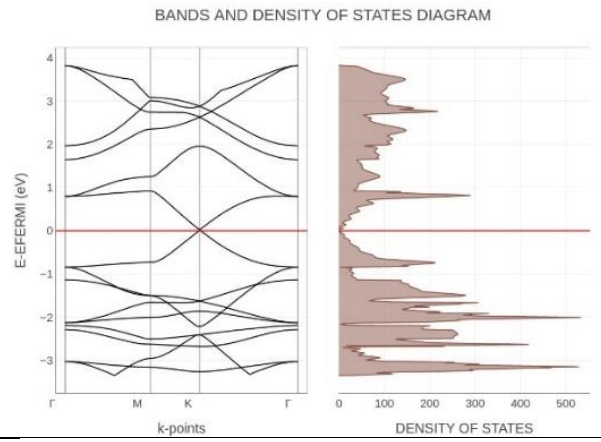
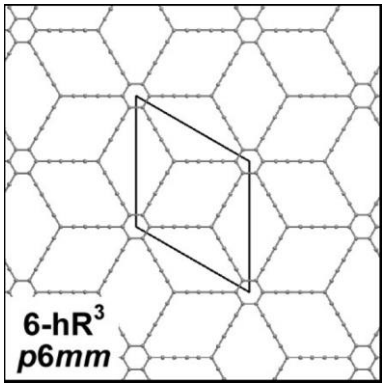
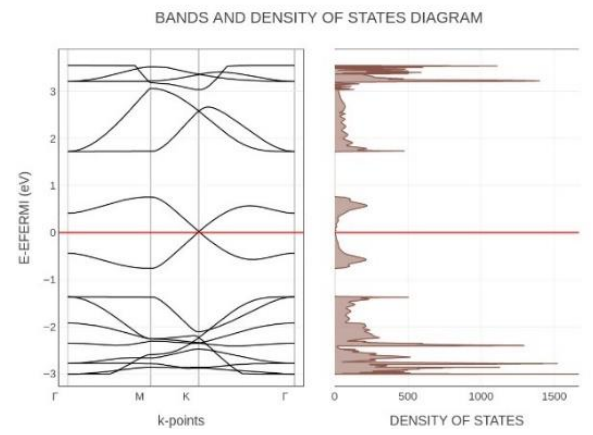
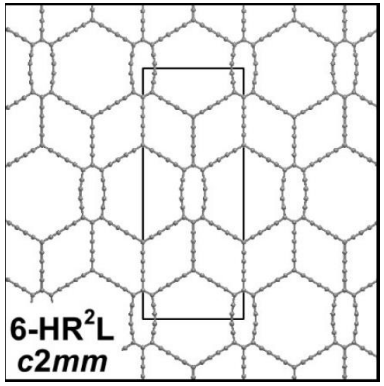
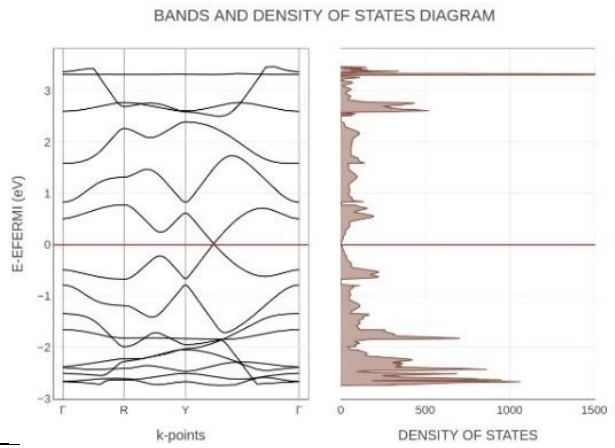
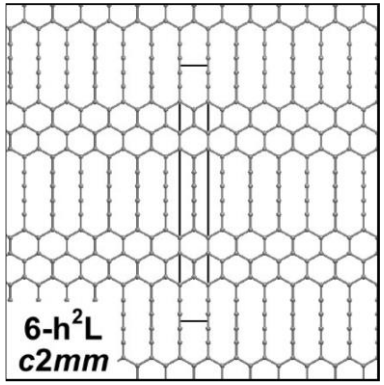
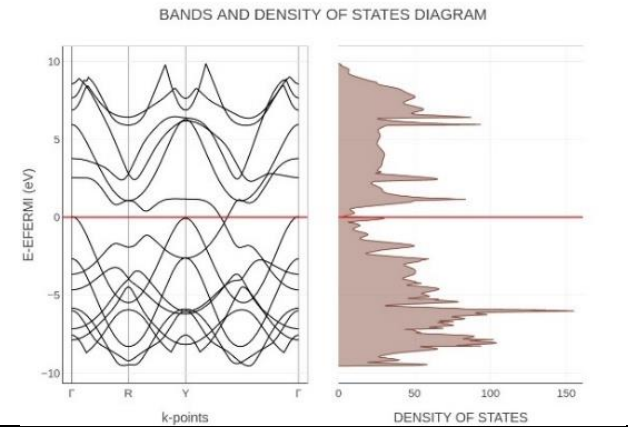
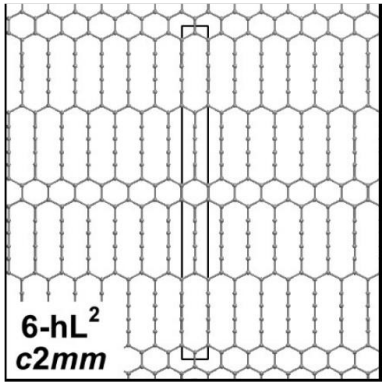
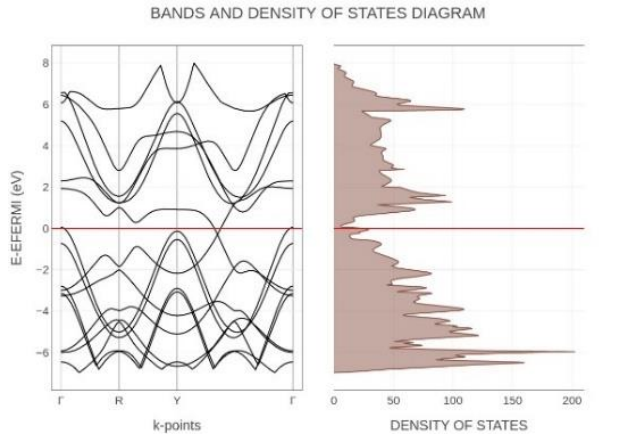
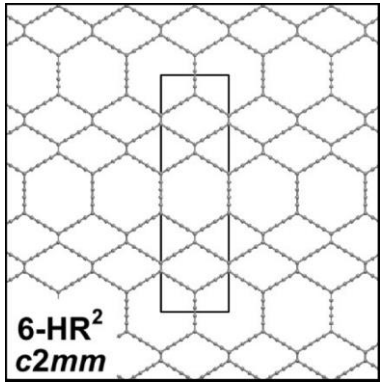
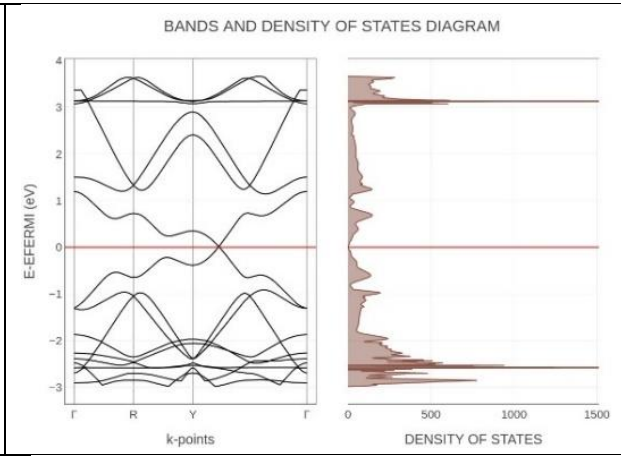
E-EFERMI (eV)
k-points
DENSITY OF STATES

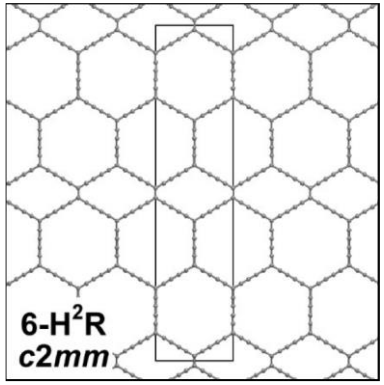
 6-hL3 p2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	
 6-HR3 p2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	
 6-H3R p2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	

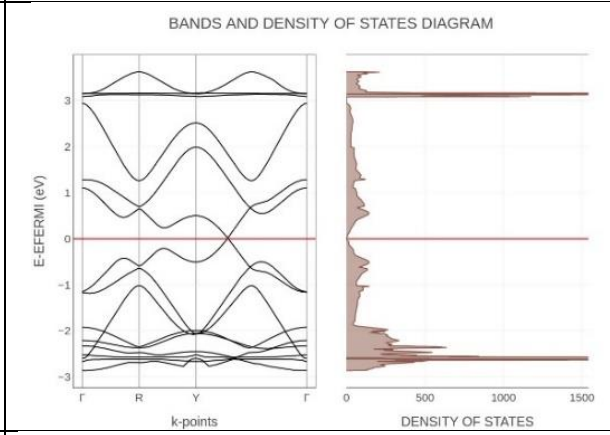
 6-hRL2 c2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) Γ R Y Γ k-points 0 50 100 150 200 250 DENSITY OF STATES	
 6-HL3 p6mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) Γ M K Γ k-points 0 100 200 300 400 500 DENSITY OF STATES	
 6-hR3 p6mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) Γ M K Γ k-points 0 500 1000 1500 DENSITY OF STATES	

 6-HR²L c2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	
 6-h²L c2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	
 6-hL² c2mm	 BANDS AND DENSITY OF STATES DIAGRAM E-EFERMI (eV) k-points DENSITY OF STATES	


6-HR²
c2mm


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ R Y Γ
k-points
0 500 1000 1500
DENSITY OF STATES


6-H²R
c2mm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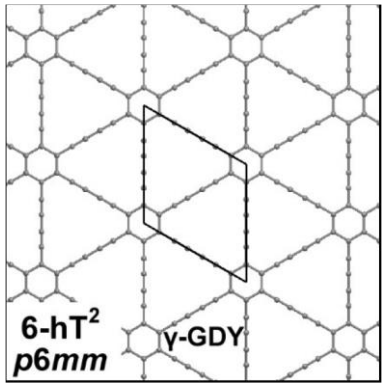
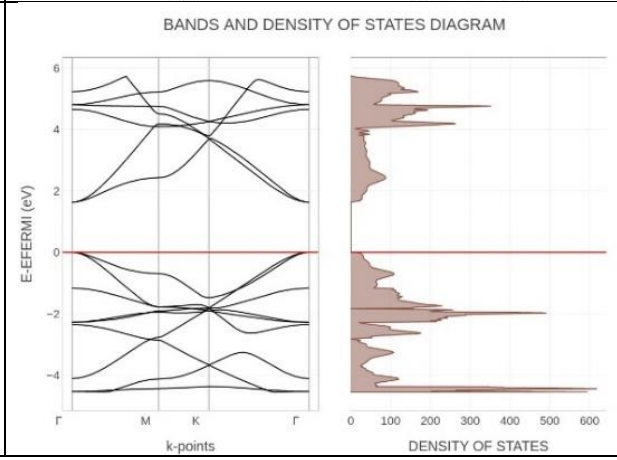
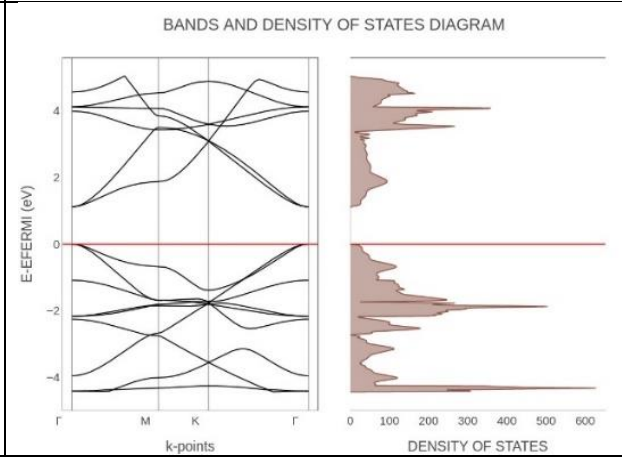
E-EFERMI (eV)
Γ R Y Γ
k-points
0 500 1000 1500
DENSITY OF STATES


6-hT²
p6mm
γ-GDY


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ M K Γ
k-points
0 100 200 300 400 500 600
DENSITY OF STATES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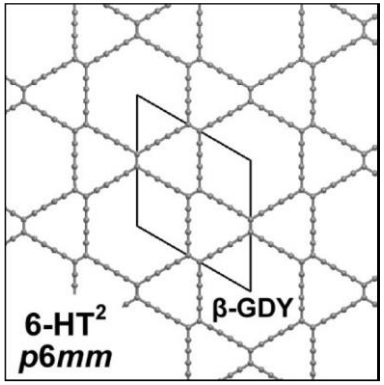
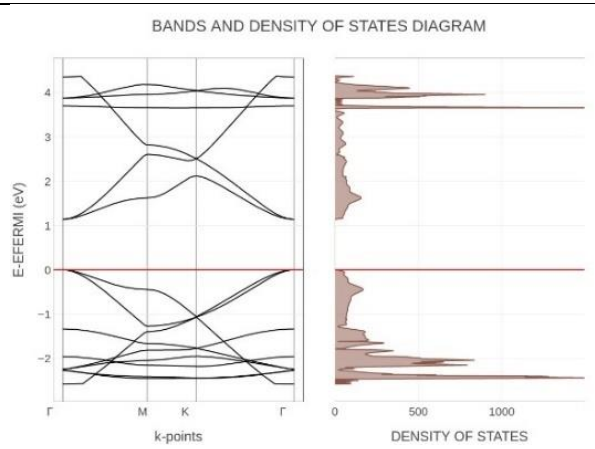
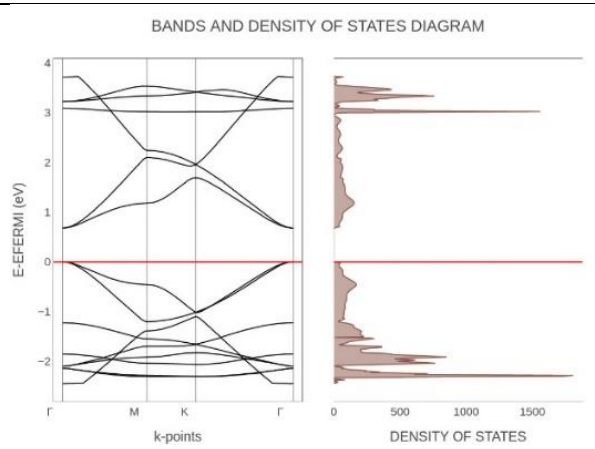
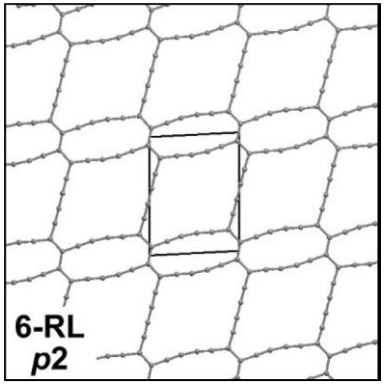
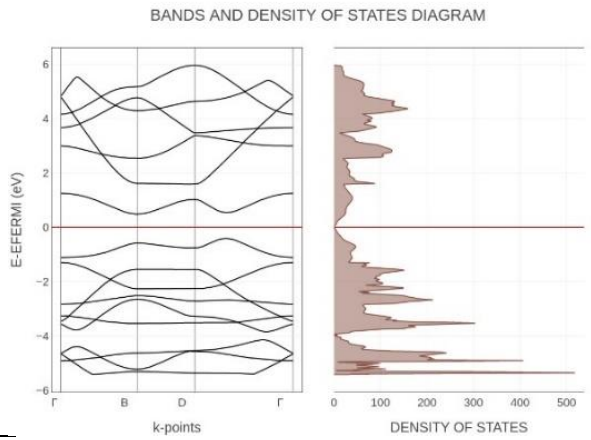
E-EFERMI (eV)
Γ M K Γ
k-points
0 100 200 300 400 500 600
DENSITY OF STATES

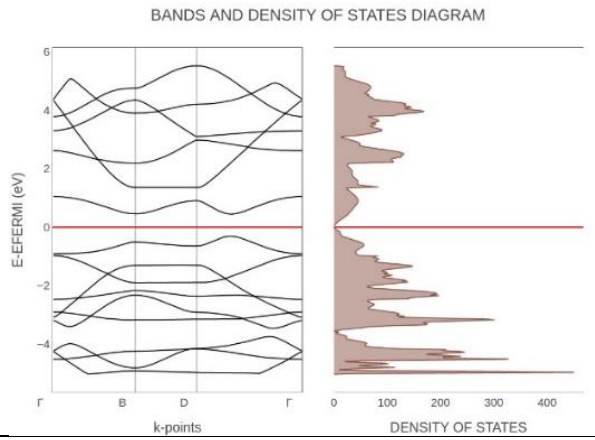

6-HT²
p6mm
β-GDY

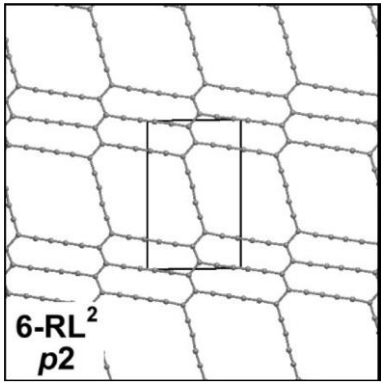

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ M K Γ
k-points
0 500 1000
DENSITY OF STATES

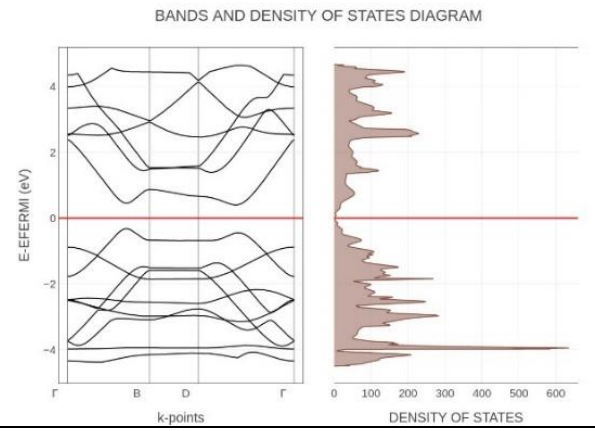

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ M K Γ
k-points
0 500 1000 1500
DENSITY OF STATES

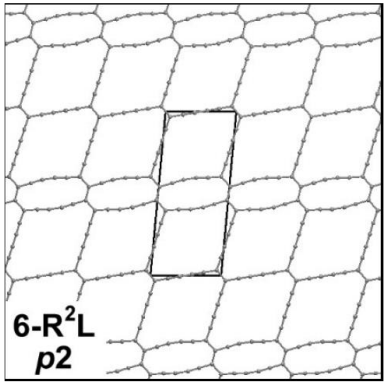

6-RL
p2

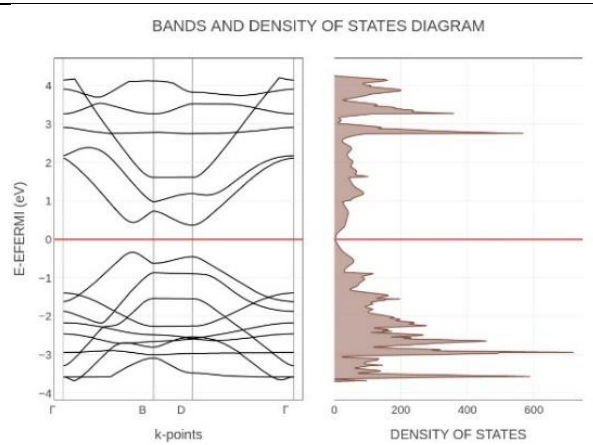

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ B D Γ
k-points
0 100 200 300 400 500
DENSITY OF STATES

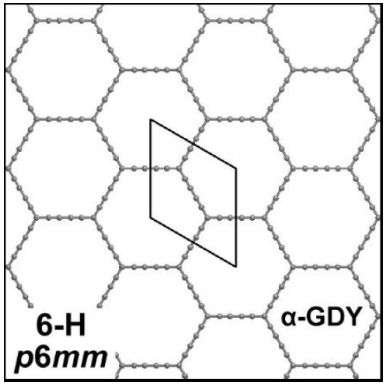

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ B D Γ
k-points
0 100 200 300 400
DENSITY OF STATES

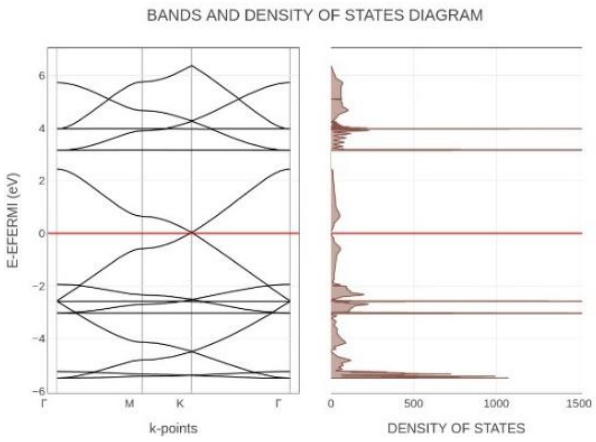

6-RL²
p2

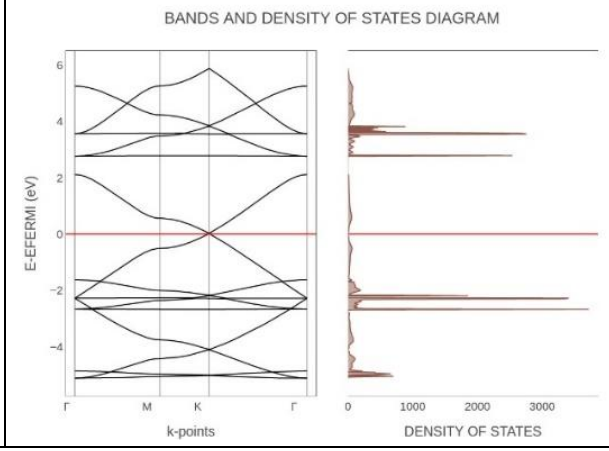

BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ B D Γ
k-points
0 100 200 300 400 500 600
DENSITY OF STATES


6-R²L
p2


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ B D Γ
k-points
0 200 400 600
DENSITY OF STATES


6-H
p6mm
α-GDY


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ M K Γ
k-points
0 500 1000 1500
DENSITY OF STATES


BANDS AND DENSITY OF STATES DIAGRAM
E-EFERMI (eV)
Γ M K Γ
k-points
0 1000 2000 3000
DENSITY OF STATES

# in Tab 1	in red the new ones	Rel Energy kcal/mol	Area (Graphene 5.26Å^2)	density atomi/angs^2 graphene 0.380	SPGR	Plane group	C(sp2)m X(sp)n	ratio sp/sp2	Z	Pearson Symbol	# of C sp2 in the primitive cell	RINGS in the primitive cell	Other names	JETP 2015 (ref. 16) JPCC 2019 grazynes (ref. 56)	npj Comp Mat 2018 (ref. 17)	Phys. Status Solidi RRL 2020 (ref. 18)	J Chem Phys 1987 (ref.15)
1	6-h^{3}L	**14,15**	34,5	0,348	Pmmm	p2mm	C X2	**0,5**	4	oP12	8	[6]$_3$[14]		**[3],[2]-grazyne = 4-h^{3}L**			
2	6-h^{2}L	**16,81**	58,2	0,344	Cmmm	c2mm	C2 X3	**0,66**	4	oS20	6	[6]$_2$[14]		**[2],[2]-grazyne = 4-h^{2}L**			
3	6-h^{2}L^2	**20,55**	48,6	0,329	Pmma	p2mg	C X	**1**	8	oP16	8	[6]$_2$[14]$_2$					
4	6-hL	**20,59**	24,3	0,330	Pmmm	p2mm	C X	**1**	4	oP8	4	[6][14]		**[1],[2]-grazyne = 4-hL**			
5	**6-hT^2**	**21,13**	77,1	0,233	P6/mmm	p6mm	C2 X	**2**	6	hP18	6	[6][18]$_2$	**γ-GDY graphdyne**	**γ1-graphyne-2**	**6-hT^2**	**191-E6Y12-1**	**6,6,6- = 4-hT^2 6,6,6-GDY**
6	6-hRL^2	**22,65**	191,9	0,250	Cmmm	c2mm	C2 X	**2**	16	oS48	8	[6][14]$_2$[22]					
7	**6-hT^{2}R**	**22,69**	131,1	0,214	Pmmm	p2mm	C5 X2	**2,5**	4	oP28	8	[6][18]$_2$[22]		**β2-γ2-graphyne = 4-hT^{2}R**	**6-hT^{2}R**	**47-E8Y20-0**	**6,6,12- = 4-hT^{2}R 6,6,18-GDY**
8	6-hL^2	**23,11**	87,3	0,321	Cmmm	c2mm	C4 X3	**1,33**	4	oS28	6	[6][14]$_2$			**>25Å**		
9	6-hL^3	**24,06**	63,1	0,317	Pmmm	p2mm	C3 X2	**1,5**	4	oP20	8	[6][14]$_3$					
10	**6-hR^3**	**24,07**	166,5	0,192	P6/mmm	p6mm	C3 X	**3**	8	hP32	8	[6][22]$_3$			**6-hR^3**	**191-E12Y12-1**	
11	6-RL^2	**24,73**	87,2	0,252	P2/m	p2	C8 X3	**2,66**	2	mP22	6	[14]$_2$[22]					
12	6-RL	**24,73**	72,7	0,220	P2/m	p2	C3 X	**3**	4	mP16	4	[14][22]					
13	6-R^{2}L	**25,03**	127,2	0,204	P2/m	p2	C10 X3	**3,33**	2	mP26	6	[14][22]$_2$					
14	6-HT^{2}L	**25,07**	202,4	0,178	Pmmm	p2mm	C7 X2	**3,5**	4	oP36	8	[14][18]$_2$[30]	**δ-GDY**	**β1-γ2-graphyne = 4-HT^{2}L**	**[4-HT^{2}L]**		
15	**6-HT^2**	**25,4**	184,6	0,163	P6/mmm	p6mm	C4 X	**4**	6	hP30	6	[18]$_2$[30]	**β-GDY**	**β1-graphyne-2**	**6-HT^2**	**191-E6Y24-1**	**12,12,12- = 4-HT^2 18,18,18-GDY**
16	**6-HL^3**	**25,41**	165,6	0,193	P6/mmm	p6mm	C3 X	**3**	8	hP32	8	[14]$_3$[30]			**[4-HL^3]**	**191-E8Y24-1**	
17	**6-R**	**25,48**	109,4	0,183	Cmmm	c2mm	C4 X	**4**	4	oS20	2	[22]	**carbon ene-yne CEY**	**β2-graphyne-2**	**6-R**	**65-E4Y16-0**	**14,14,14- = 4-R 22,22,22-GDY**
18	6-HR^{2}L	**25,85**	474,9	0,168	Cmmm	c2mm	C4 X	**4**	16	oS80	8	[14][22]$_2$[30]			**>25Å**		
19	6-HR^3	**26,11**	276,1	0,159	Pmmm	p2mm	C9 X2	**4,5**	4	oP44	8	[22]$_3$[30]			**>25Å**		
20	**6-L**	**26,18**	38,9	0,309	Cmmm	c2mm	C2 X	**2**	4	oS12	2	[14]		**γ2-graphyne-2**		**65-E4Y8-0 γ2-graphdiyne**	
21	6-HR^2	**26,3**	442,5	0,154	Cmmm	c2mm	C14 X3	**4,66**	4	oS68	6	[22]2[30]		**α-β2-graphyne Fig 4b = 4-HR^2**	**>25Å**		
22	**6-HR**	**26,63**	166,7	0,144	Pmmm	p2mm	C5 X	**5**	4	oP24	4	[22][30]		**α-β2-graphyne Fig 4a = 4-HR**	**6-HR**	**47-E4Y20-0**	**14,14,18- = 4-HR 22,22,30-GDY**
23	6-H^{2}R^2	**26,63**	333,5	0,144	Pmma	p2mg	C5 X	**5**	8	oP48	8	[22]$_2$[30]$_2$			**>25Å**		
24	6-H^{2}R	**26,92**	558,2	0,136	Cmmm	c2mm	C16 X3	**5,33**	4	oS76	6	[22][30]$_2$			**>25Å**		
25	6-H^{3}R	**27,05**	391,5	0,133	Pmmm	p2mm	C11 X2	**5,5**	4	oP52	8	[22][30]$_3$			**>25Å**		
26	**6-H**	**27,39**	112,5	0,124	P6/mmm	p6mm	C6 X	**6**	2	hP14	2	[30]	**α-GDY**	**α-graphyne-2**	**6-H**	**191-E2Y22-0**	**18,18,18- = 4-H 30,30,30-GDY**

***Table S2**:* Crystallographic informations for all the 26 2D GDY-based crystals investigated in the work