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RESEARCH ARTICLE

Interlayer interaction mechanism and its regulation on optical properties of bilayer SiCNSs

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Supplementary Information

Table S1 Charge distribution in the ML-SiCNSs.

Atom	Charge (e)	Fractional coordinates of atoms			Atom	Charge (e)	Fractional coordinates of atoms		
		u	*v*	*w*			*u*	*v*	*w*
C1	-1.46	0.166667	0.083333	0.495327	Si1	+1.46	0.083333	0.166667	0.496705
C2	-1.46	0.416666	0.083333	0.495329	Si2	+1.46	0.333333	0.166667	0.496706
C3	-1.46	0.666667	0.083333	0.495322	Si3	+1.46	0.583333	0.166667	0.496704
C4	-1.46	0.916667	0.083333	0.495328	Si4	+1.46	0.833333	0.166667	0.496704
C5	-1.46	0.166667	0.333333	0.495328	Si5	+1.46	0.083333	0.416667	0.496706
C6	-1.46	0.416667	0.333333	0.495328	Si6	+1.46	0.333333	0.416667	0.496706
C7	-1.46	0.666667	0.333334	0.495327	Si7	+1.46	0.583333	0.583333	0.496705
C8	-1.46	0.916667	0.333334	0.495328	Si8	+1.46	0.833333	0.416667	0.496706
C9	-1.46	0.166667	0.583333	0.495327	Si9	+1.46	0.083333	0.666667	0.496706
C10	-1.46	0.416667	0.583333	0.495329	Si10	+1.46	0.333333	0.666667	0.496706
C11	-1.46	0.666667	0.583333	0.495326	Si11	+1.46	0.583333	0.666667	0.496705
C12	-1.46	0.916667	0.583334	0.495329	Si12	+1.46	0.833333	0.666667	0.496706
C13	-1.46	0.166666	0.833333	0.495329	Si13	+1.46	0.083333	0.916667	0.496706
C14	-1.46	0.416666	0.833333	0.495328	Si14	+1.46	0.333333	0.916667	0.496706
C15	-1.46	0.666667	0.833333	0.495328	Si15	+1.46	0.583333	0.916667	0.496704
C16	-1.46	0.916667	0.833333	0.495329	Si16	+1.46	0.833333	0.916667	0.496706

Table S2 Charge distribution in the bilayer-T.

Atom	Charge (e)	Fractional coordinates of atoms			Atom	Charge (e)	Fractional coordinates of atoms		
		u	*v*	*w*			*u*	*v*	*w*
C1	-1.44	0.085846	0.082232	0.396853	Si17	+1.44	0.168991	0.91566	0.397241
C3	-1.44	0.335846	0.832232	0.396853	Si18	+1.44	0.418991	0.66566	0.397241
C5	-1.44	0.585846	0.582232	0.396853	Si19	+1.44	0.668991	0.41566	0.397241
C7	-1.44	0.835846	0.332232	0.396853	Si20	+1.44	0.918991	0.16566	0.397241
C9	-1.44	0.085846	0.332232	0.396853	Si21	+1.44	0.168991	0.16566	0.397241
C11	-1.44	0.335846	0.082232	0.396853	Si22	+1.44	0.418991	0.91566	0.397241
C13	-1.44	0.585846	0.832232	0.396853	Si23	+1.44	0.668991	0.66566	0.397241
C15	-1.44	0.835846	0.582232	0.396853	Si24	+1.44	0.918991	0.41566	0.397241
C17	-1.44	0.085846	0.582232	0.396853	Si25	+1.44	0.168991	0.41566	0.397241
C19	-1.44	0.335846	0.332232	0.396853	Si26	+1.44	0.418991	0.16566	0.397241
C21	-1.44	0.585846	0.082232	0.396853	Si27	+1.44	0.668991	0.91566	0.397241
C23	-1.44	0.835846	0.832232	0.396853	Si28	+1.44	0.918991	0.66566	0.397241
C25	-1.44	0.085846	0.832232	0.396853	Si29	+1.44	0.168991	0.66566	0.397241
C27	-1.44	0.335846	0.582232	0.396853	Si30	+1.44	0.418991	0.41566	0.397241
C29	-1.44	0.585846	0.332232	0.396853	Si31	+1.44	0.668991	0.16566	0.397241
C31	-1.44	0.835846	0.082232	0.396853	Si32	+1.44	0.918991	0.91566	0.397241

Table S3 Charge distribution in the bilayer-B.

Atom	Charge (e)	Fractional coordinates of atoms			Atom	Charge (e)	Fractional coordinates of atoms		
		u	*v*	*w*			*u*	*v*	*w*
C1	-1.44	0.168959	0.915789	0.594914	Si17	+1.44	0.08561	0.082455	0.594517
C3	-1.44	0.418959	0.665789	0.594914	Si18	+1.44	0.33561	0.832455	0.594517
C5	-1.44	0.668959	0.415789	0.594914	Si19	+1.44	0.58561	0.582455	0.594517
C7	-1.44	0.918959	0.165789	0.594914	Si20	+1.44	0.83561	0.332455	0.594517
C9	-1.44	0.168959	0.165789	0.594914	Si21	+1.44	0.08561	0.332455	0.594517
C11	-1.44	0.418959	0.915789	0.594914	Si22	+1.44	0.33561	0.082455	0.594517
C13	-1.44	0.668959	0.665789	0.594914	Si23	+1.44	0.58561	0.832455	0.594517
C15	-1.44	0.918959	0.415789	0.594914	Si24	+1.44	0.83561	0.582455	0.594517
C17	-1.44	0.168959	0.415789	0.594914	Si25	+1.44	0.08561	0.582455	0.594517
C19	-1.44	0.418959	0.165789	0.594914	Si26	+1.44	0.33561	0.332455	0.594517
C21	-1.44	0.668959	0.915789	0.594914	Si27	+1.44	0.58561	0.082455	0.594517
C23	-1.44	0.918959	0.665789	0.594914	Si28	+1.44	0.83561	0.832455	0.594517
C25	-1.44	0.168959	0.665789	0.594914	Si29	+1.44	0.08561	0.832455	0.594517
C27	-1.44	0.418959	0.415789	0.594914	Si30	+1.44	0.33561	0.582455	0.594517
C29	-1.44	0.668959	0.165789	0.594914	Si31	+1.44	0.58561	0.332455	0.594517
C31	-1.44	0.918959	0.915789	0.594914	Si32	+1.44	0.83561	0.082455	0.594517

Table S4 Interlayer coupling energy and interlayer force of bilayer SiCNSs.

SiCNSs	Spacing *r*(Å)	Total energy(eV)	Coupling energy(eV)	Interlayer force(eV/Å)	Spacing *r*(Å)	Total energy(eV)	Coupling energy(eV)	Interlayer force(eV/Å)
Monolayer	0	-4190.395	——	——	2.8	-8389.642	-8.851	-1.686
Bilayer	2.0	-8385.145	-4.354	27.064	2.9	-8389.461	-8.670	-1.741
	2.1	-8387.851	-7.060	20.375	3.0	-8389.293	-8.502	-1.389
	2.2	-8389.220	-8.429	9.968	3.5	-8388.745	-7.954	-1.528
	2.3	-8389.845	-9.054	4.429	4.0	-8387.765	-6.974	-2.212
	2.4	-8390.106	-9.315	1.316	4.5	-8386.533	-5.742	-1.967
	2.5	-8390.108	-9.317	-0.684	5.0	-8385.798	-5.007	-1.201
	2.6	-8389.969	-9.178	-1.548	5.5	-8385.333	-4.542	-0.718
	2.7	-8389.799	-9.008	-1.636	6.0	-8385.080	-4.289	-0.506

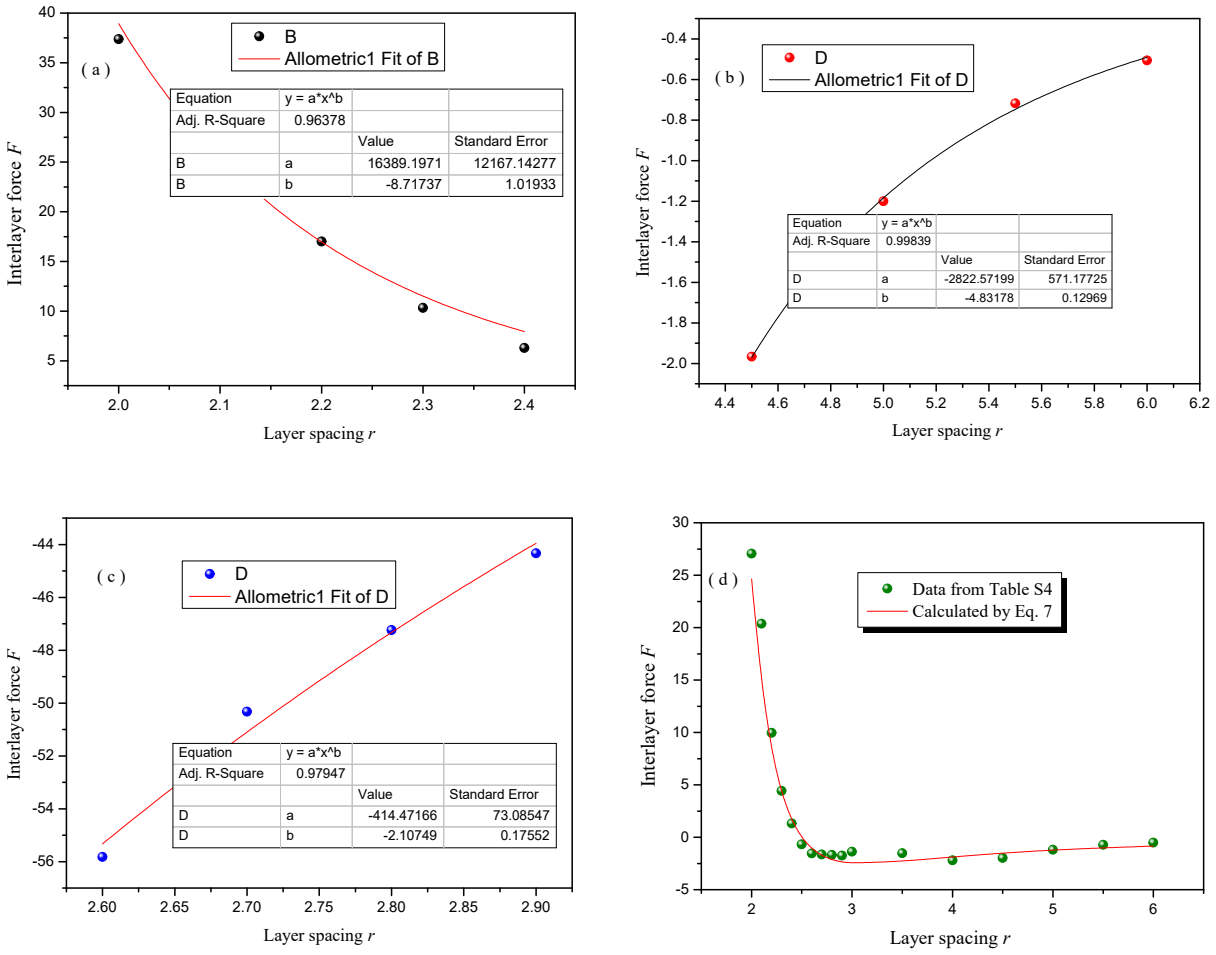
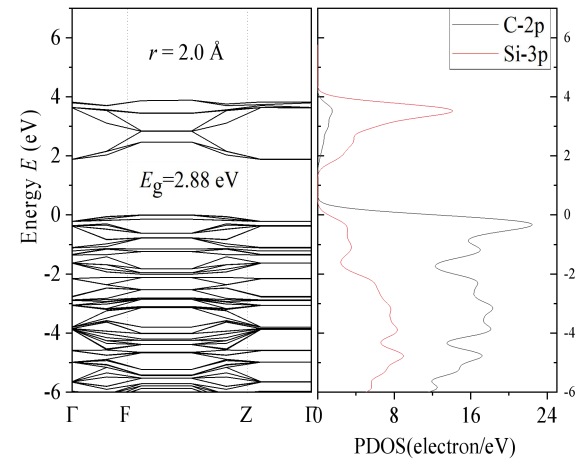
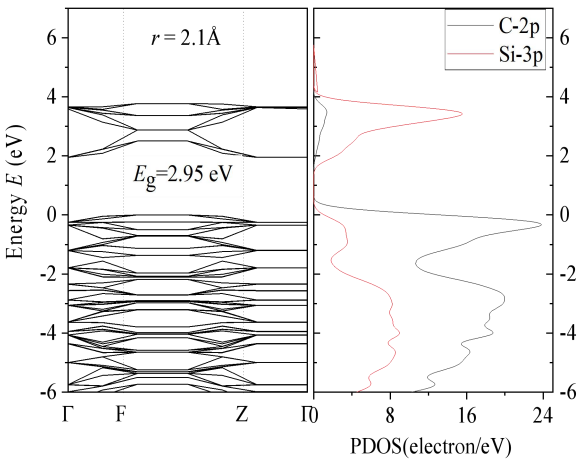


Fig. S1 Interlayer force fitting of bilayer SiCNSs.

Table S5 Bond population of BL-SiCNSs.

	Layer inside		Between layers					
	Si-C(Å)	Population	Si-C(Å)	Population	Si-Si(Å)	Population	C-C(Å)	Population
2.0	1.78	0.81	2.00	0.31	2.67	-0.15	2.67	-0.35
2.1	1.78	0.84	2.10	0.24	2.75	-0.12	2.75	-0.30
2.2	1.78	0.86	2.20	0.18	2.83	-0.09	2.83	-0.26
2.3	1.78	0.88	2.30	0.13	2.90	-0.08	2.90	-0.22
2.4	1.78	0.90	2.40	0.09	2.94	-0.06	2.99	-0.19
2.5	1.78	0.91	2.50	0.06	—	—	—	—
2.6	1.78	0.92	2.60	0.04	—	—	—	—
2.7	1.78	0.93	2.70	0.02	—	—	—	—
2.8	1.78	0.93	2.80	0.01	—	—	—	—
2.9	1.78	0.94	2.90	-0.01	—	—	—	—
3.0	1.78	0.94	—	—	—	—	—	—
3.5	1.78	0.94	—	—	—	—	—	—
4.0	1.78	0.94	—	—	—	—	—	—
4.5	1.78	0.94	—	—	—	—	—	—
5.0	1.78	0.93	—	—	—	—	—	—
5.5	1.78	0.93	—	—	—	—	—	—
6.0	1.78	0.93	—	—	—	—	—	—


r = 2.0 Å
Eg=2.88 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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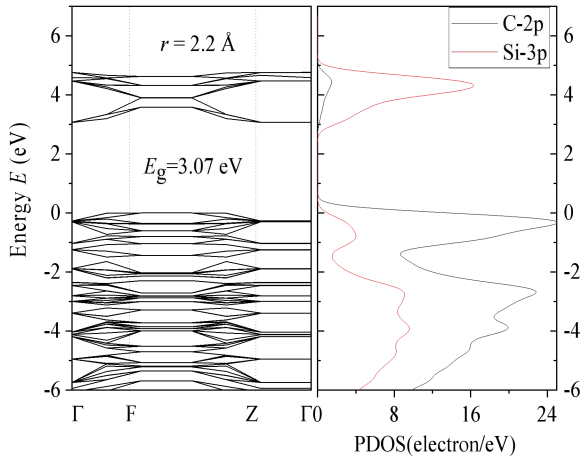
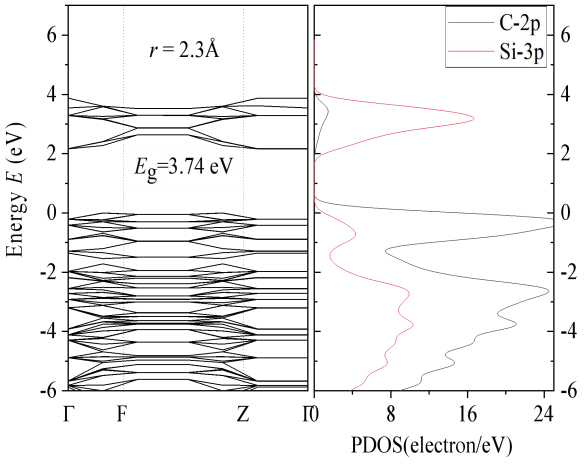
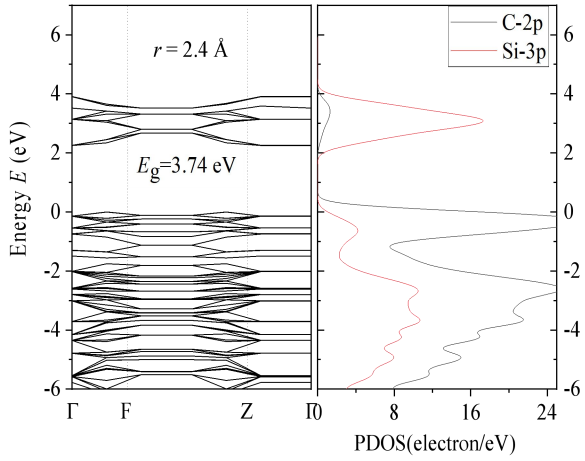
Eg=2.95 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)


r = 2.2 Å
Eg=3.07 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)


r = 2.3Å
Eg=3.74 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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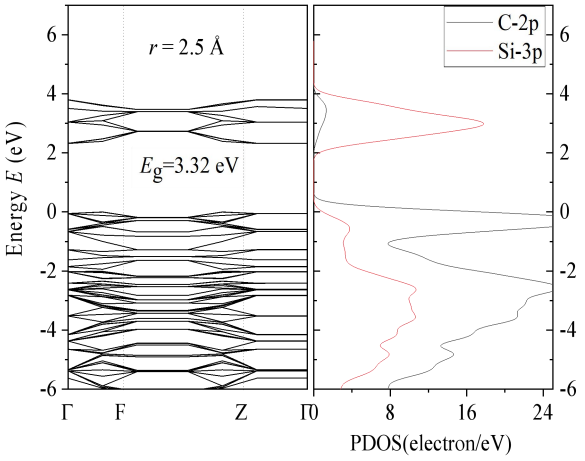
Eg=3.74 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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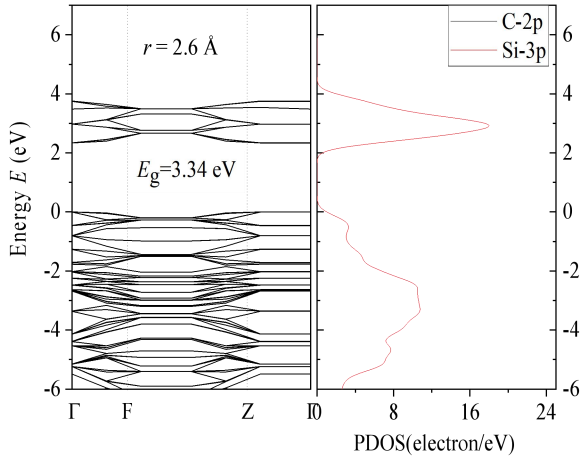
Eg=3.32 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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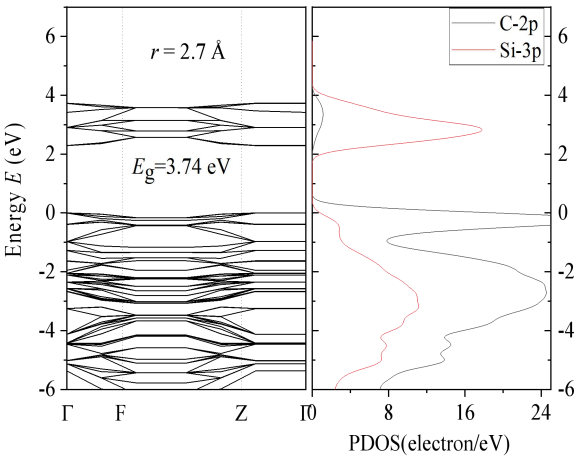
Eg=3.34 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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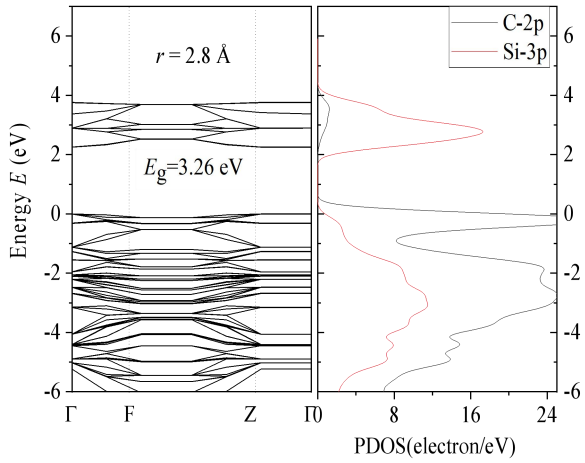
Eg=3.74 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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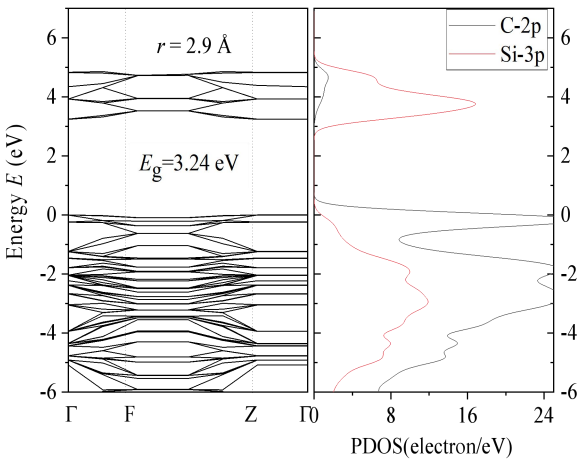
Eg=3.26 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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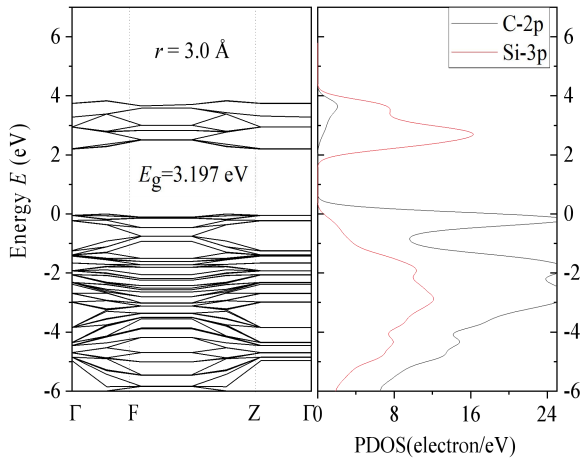
Eg=3.24 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)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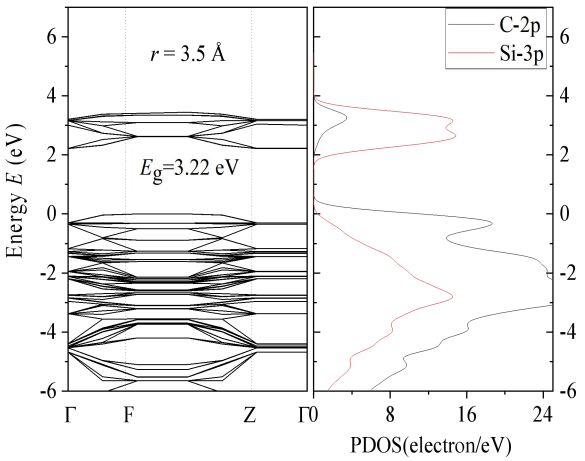
Γ F Z Γ0
PDOS(electron/eV)


r = 3.5 Å
Eg=3.22 eV
C-2p
Si-3p
Energy E (eV)
Γ F Z Γ0
PDOS(electron/eV)

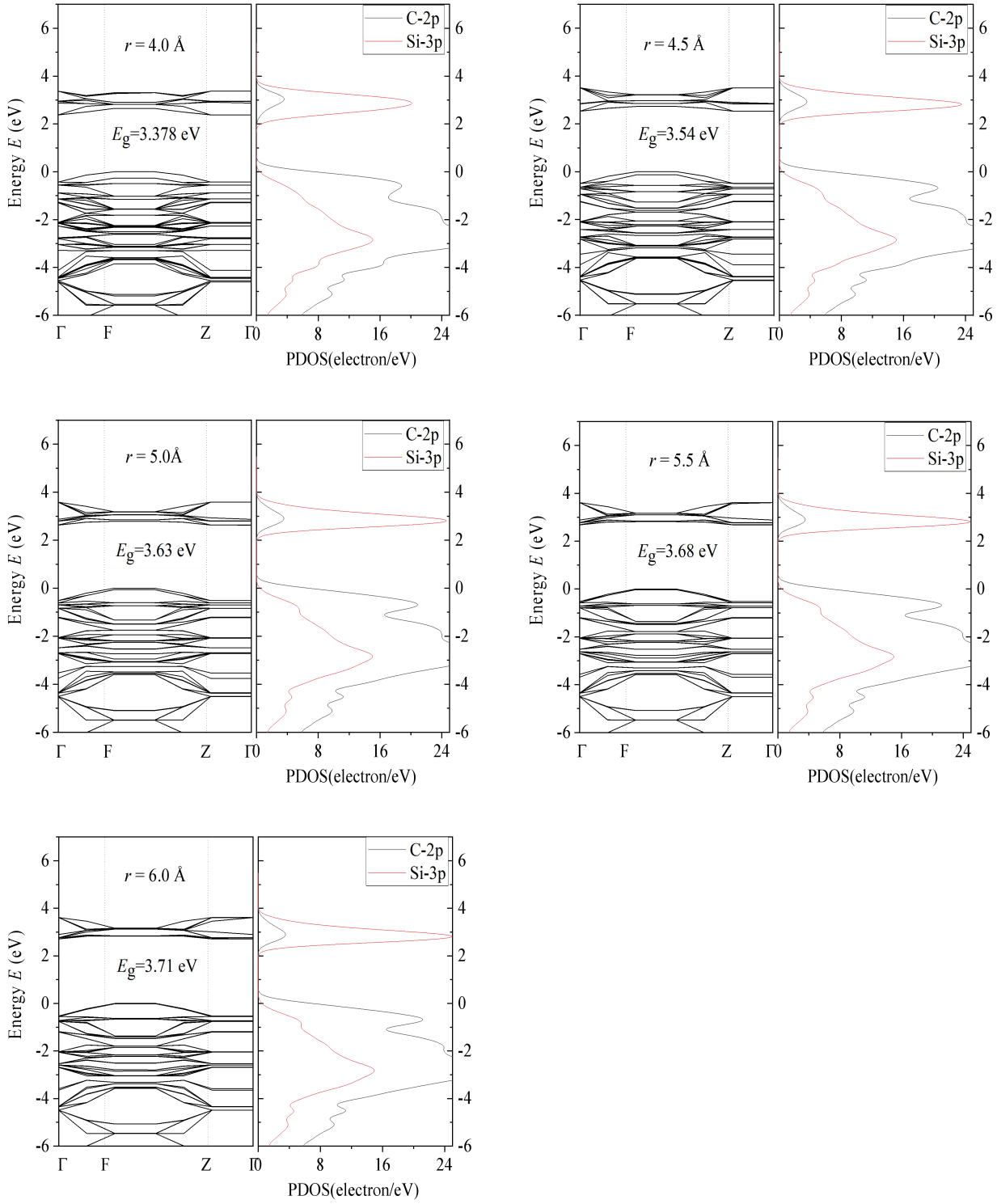


Fig. S2 The energy band and state density of BL-SiCNSs at different interlayer distances.