SUPPLEMENTAL MATERIAL: Insights into the adhesion and delamination strength of carbon films on metals by high-throughput *ab initio* calculations

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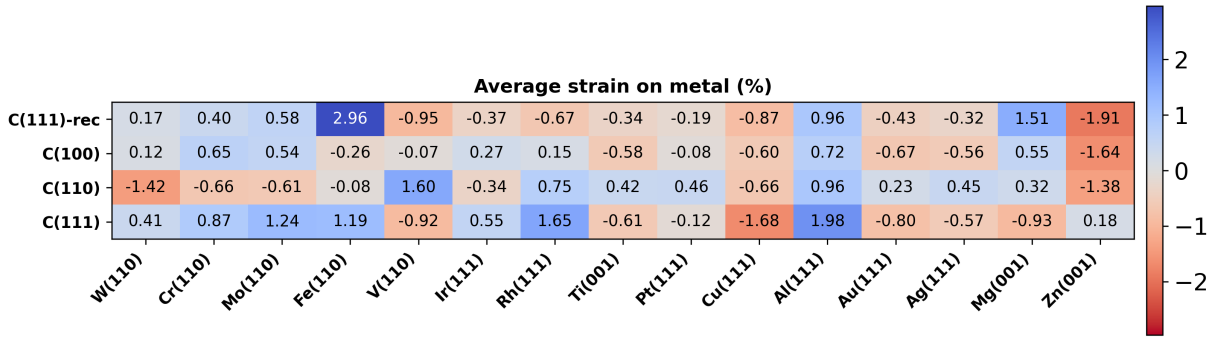
1. Computational parameters

Material	E_{cut} (eV)	Kdens (1/Å)	(hkl)	layers
W	225	8.1	(110)	4
Cr	300	3.9	(110)	6
Mo	250	6.3	(110)	4
Fe	325	4.0	(110)	4
V	300	5.3	(110)	4
Ir	225	7.7	(111)	3
Rh	275	4.4	(111)	3
Ti	250	3.5	(001)	6
Pt	250	6.1	(111)	4
Cu	375	4.2	(111)	4
Al	275	6.6	(111)	5
Ag	300	4.4	(111)	12
Au	275	5.2	(111)	7
Mg	400	6.5	(001)	7
Zn	275	6.0	(001)	12
C	400	4.0	(111)-rec	10
		4.0	(100)	10
		3.2	(110)	8
		3.2	(111)	8

TABLE I. Converged values of cutoff energies, k-point densities and number of layers of the selected surface terminations obtained with the workflow implemented in TribChem.

2. Average strain on metal



(a)

FIG. 1. Average percentage strain applied on the metal constituent in the interface supercell. Negative values correspond to compressive strain (red regions), whereas positive values represent tensile strain (blue regions).

3. Supercell construction

The interface supercells were constructed starting from the 2D surface lattices of the diamond and metal slabs. For each pair, the lattice matching was optimized using the Zur and McGill algorithm, which searches for commensurate supercells that minimize the interfacial strain. The resulting transformation matrices are summarized in Tables II–V.

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For both the diamond and metal slabs, the table reports the transformation matrix T that converts the primitive 2D lattice vectors of the slab into those of the interface supercell ($L_{\text{super}} = TL_{\text{slab}}$). Through polar decomposition, T can be expressed as $T = RS$, where R is a rotation matrix and S is a symmetric positive-definite scaling matrix. The corresponding rotation angles (in degrees) are also reported. When the rotation is zero, the scaling matrix S coincides with T.

Diamond	Metal	Transformation on Diamond lattice			Transformation on Metal lattice		
		T	S	Rotation (°)	T	S	Rotation (°)
C(111)-rec	W	$\begin{pmatrix} 2.07 & 0 \\ 0 & 6.28 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.30 & 2.03 \\ 0 & 6.09 \end{pmatrix}$	$\begin{pmatrix} 3.21 & 0.69 \\ 0.69 & 6.38 \end{pmatrix}$	-12.22
	Cr	$\begin{pmatrix} 5.72 & 0 \\ 0 & 13.88 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.01 & 4.99 \\ 0 & 14.97 \end{pmatrix}$	$\begin{pmatrix} 0.96 & 0.30 \\ 0.30 & 15.78 \end{pmatrix}$	-17.34
	Mo	$\begin{pmatrix} 2.06 & 0 \\ 0 & 6.25 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.30 & 2.04 \\ 0 & 6.12 \end{pmatrix}$	$\begin{pmatrix} 3.22 & 0.70 \\ 0.70 & 6.41 \end{pmatrix}$	-12.22
	Fe	$\begin{pmatrix} 2.31 & 1.15 \\ 0 & 3.46 \end{pmatrix}$	$\begin{pmatrix} 2.26 & 0.45 \\ 0.45 & 3.62 \end{pmatrix}$	-11.31	$\begin{pmatrix} 4.12 & 3.32 \\ 0 & 3.78 \end{pmatrix}$	$\begin{pmatrix} 3.80 & 1.60 \\ 1.60 & 4.77 \end{pmatrix}$	-22.79
	V	$\begin{pmatrix} 0.59 & 0 \\ 0 & 8.69 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.99 & 2.99 \\ 0 & 8.96 \end{pmatrix}$	$\begin{pmatrix} 0.94 & 0.28 \\ 0.28 & 9.44 \end{pmatrix}$	-16.72
	Ir	$\begin{pmatrix} 2.52 & 0.13 \\ 0 & 5.56 \end{pmatrix}$	$\begin{pmatrix} 2.52 & 0.04 \\ 0.04 & 5.56 \end{pmatrix}$	-0.94	$\begin{pmatrix} 4.02 & -2.75 \\ 0 & 5.92 \end{pmatrix}$	$\begin{pmatrix} 3.87 & -1.07 \\ -1.07 & 6.44 \end{pmatrix}$	15.46
	Rh	$\begin{pmatrix} 3.08 & 1.54 \\ 0 & 4.61 \end{pmatrix}$	$\begin{pmatrix} 3.02 & 0.60 \\ 0.60 & 4.83 \end{pmatrix}$	-11.31	$\begin{pmatrix} 4.97 & 0 \\ 0 & 4.97 \end{pmatrix}$	–	0
	Ti	$\begin{pmatrix} 1.16 & 0.58 \\ 0 & 1.74 \end{pmatrix}$	$\begin{pmatrix} 1.14 & 0.23 \\ 0.23 & 1.82 \end{pmatrix}$	-11.31	$\begin{pmatrix} 1.73 & 0 \\ 0 & 1.73 \end{pmatrix}$	–	0
	Pt	$\begin{pmatrix} 2.31 & 1.15 \\ 0 & 3.46 \end{pmatrix}$	$\begin{pmatrix} 2.26 & 0.45 \\ 0.45 & 3.62 \end{pmatrix}$	-11.31	$\begin{pmatrix} 3.60 & 0 \\ 0 & 3.60 \end{pmatrix}$	–	0
	Cu	$\begin{pmatrix} 0.58 & 0 \\ 0 & 1.75 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.99 & -0.99 \\ 0 & 1.98 \end{pmatrix}$	$\begin{pmatrix} 0.94 & -0.31 \\ -0.31 & 2.19 \end{pmatrix}$	18.43
	Al	$\begin{pmatrix} 1.14 & 0.57 \\ 0 & 1.72 \end{pmatrix}$	$\begin{pmatrix} 1.12 & 0.22 \\ 0.22 & 1.79 \end{pmatrix}$	-11.31	$\begin{pmatrix} 1.75 & 0 \\ 0 & 1.75 \end{pmatrix}$	–	0
	Ag	$\begin{pmatrix} 1.15 & 0.58 \\ 0 & 1.74 \end{pmatrix}$	$\begin{pmatrix} 1.14 & 0.23 \\ 0.23 & 1.82 \end{pmatrix}$	-11.31	$\begin{pmatrix} 1.73 & 0 \\ 0 & 1.73 \end{pmatrix}$	–	0
	Au	$\begin{pmatrix} 1.16 & -0.58 \\ 0 & 1.74 \end{pmatrix}$	$\begin{pmatrix} 1.14 & -0.23 \\ -0.23 & 1.82 \end{pmatrix}$	11.31	$\begin{pmatrix} 1.72 & 0 \\ 0 & 1.72 \end{pmatrix}$	–	0
	Mg	$\begin{pmatrix} 1.97 & 0.99 \\ 0 & 2.96 \end{pmatrix}$	$\begin{pmatrix} 1.93 & 0.39 \\ 0.39 & 3.09 \end{pmatrix}$	-11.31	$\begin{pmatrix} 2.69 & 0 \\ 0 & 2.69 \end{pmatrix}$	–	0
	Zn	$\begin{pmatrix} 0.59 & 0 \\ 0 & 1.77 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.98 & -0.98 \\ 0 & 1.96 \end{pmatrix}$	$\begin{pmatrix} 0.93 & -0.31 \\ -0.31 & 2.17 \end{pmatrix}$	18.43

TABLE II. Transformations used to construct C(111)-rec/metal interface supercells.

Diamond	Metal	Transformation on Diamond lattice			Transformation on Metal lattice		
		T	S	Rotation (°)	T	S	Rotation (°)
C(100)	W	$\begin{pmatrix} 2.06 & 0.24 \\ 0 & 6.28 \end{pmatrix}$	$\begin{pmatrix} 2.06 & 0.06 \\ 0.06 & 6.29 \end{pmatrix}$	-1.66	$\begin{pmatrix} 3.78 & 2.48 \\ 0 & 6.10 \end{pmatrix}$	$\begin{pmatrix} 3.67 & 0.92 \\ 0.92 & 6.52 \end{pmatrix}$	-14.07
	Cr	$\begin{pmatrix} 2.06 & 0 \\ 0 & 6.25 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.01 & 5.02 \\ 0 & 15.05 \end{pmatrix}$	$\begin{pmatrix} 0.96 & 0.30 \\ 0.30 & 15.87 \end{pmatrix}$	-17.35
	Mo	$\begin{pmatrix} 2.06 & 0.24 \\ 0 & 6.26 \end{pmatrix}$	$\begin{pmatrix} 2.06 & 0.06 \\ 0.06 & 6.26 \end{pmatrix}$	-1.66	$\begin{pmatrix} 3.80 & 2.49 \\ 0 & 6.12 \end{pmatrix}$	$\begin{pmatrix} 3.68 & 0.92 \\ 0.92 & 6.54 \end{pmatrix}$	-14.07
	Fe	$\begin{pmatrix} 1.80 & 0.69 \\ 0 & 3.33 \end{pmatrix}$	$\begin{pmatrix} 1.79 & 0.24 \\ 0.24 & 3.39 \end{pmatrix}$	-7.70	$\begin{pmatrix} 3.71 & 2.64 \\ 0 & 3.64 \end{pmatrix}$	$\begin{pmatrix} 3.50 & 1.26 \\ 1.26 & 4.31 \end{pmatrix}$	-19.76
	V	$\begin{pmatrix} 0.99 & 0 \\ 0 & 11.07 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.93 & 3.81 \\ 0 & 11.42 \end{pmatrix}$	$\begin{pmatrix} 1.86 & 0.53 \\ 0.53 & 12.02 \end{pmatrix}$	-15.91
	Ir	$\begin{pmatrix} 2.70 & 0.27 \\ 0 & 6.63 \end{pmatrix}$	$\begin{pmatrix} 2.70 & 0.08 \\ 0.08 & 6.63 \end{pmatrix}$	-1.69	$\begin{pmatrix} 4.98 & -3.02 \\ 0 & 7.06 \end{pmatrix}$	$\begin{pmatrix} 4.83 & -1.21 \\ -1.21 & 7.58 \end{pmatrix}$	14.09
	Rh	$\begin{pmatrix} 1.10 & 0 \\ 0 & 9.12 \end{pmatrix}$	–	0	$\begin{pmatrix} 2.04 & -4.91 \\ 0 & 9.82 \end{pmatrix}$	$\begin{pmatrix} 1.89 & -0.78 \\ -0.78 & 10.95 \end{pmatrix}$	22.48
	Ti	$\begin{pmatrix} 1 & 0.50 \\ 0 & 4.03 \end{pmatrix}$	$\begin{pmatrix} 1 & 0.10 \\ 0.10 & 4.06 \end{pmatrix}$	-5.69	$\begin{pmatrix} 1.73 & -1.14 \\ 0 & 4.01 \end{pmatrix}$	$\begin{pmatrix} 1.69 & -0.34 \\ -0.34 & 4.15 \end{pmatrix}$	11.25
	Pt	$\begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.60 & -2.08 \\ 0 & 4.16 \end{pmatrix}$	$\begin{pmatrix} 3.48 & -0.93 \\ -0.93 & 4.55 \end{pmatrix}$	15
	Cu	$\begin{pmatrix} 1.01 & 0 \\ 0 & 7.02 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.98 & -3.99 \\ 0 & 7.97 \end{pmatrix}$	$\begin{pmatrix} 1.84 & -0.73 \\ -0.73 & 8.88 \end{pmatrix}$	21.82
	Al	$\begin{pmatrix} 0.99 & 0.50 \\ 0 & 3.98 \end{pmatrix}$	$\begin{pmatrix} 0.99 & 0.10 \\ 0.19 & 4.01 \end{pmatrix}$	-5.69	$\begin{pmatrix} 1.75 & -1.16 \\ 0 & 4.06 \end{pmatrix}$	$\begin{pmatrix} 1.72 & -0.34 \\ -0.34 & 4.21 \end{pmatrix}$	11.25
	Ag	$\begin{pmatrix} 1 & 0.50 \\ 0 & 4.03 \end{pmatrix}$	$\begin{pmatrix} 1 & 0.10 \\ 0.10 & 4.06 \end{pmatrix}$	-5.69	$\begin{pmatrix} 1.73 & -1.14 \\ 0 & 4.01 \end{pmatrix}$	$\begin{pmatrix} 1.69 & -0.34 \\ -0.34 & 4.14 \end{pmatrix}$	11.25
	Au	$\begin{pmatrix} 1 & 0.50 \\ 0 & 4.04 \end{pmatrix}$	$\begin{pmatrix} 1 & 0.10 \\ 0.10 & 4.07 \end{pmatrix}$	-5.69	$\begin{pmatrix} 1.72 & -1.14 \\ 0 & 4 \end{pmatrix}$	$\begin{pmatrix} 1.70 & -0.34 \\ -0.34 & 4.15 \end{pmatrix}$	11.25
	Mg	$\begin{pmatrix} 1.11 & 0 \\ 0 & 8.92 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.75 & -4.05 \\ 0 & 8.11 \end{pmatrix}$	$\begin{pmatrix} 1.61 & -0.66 \\ -0.66 & 9.04 \end{pmatrix}$	22.36
	Zn	$\begin{pmatrix} 1.02 & 0 \\ 0 & 7.10 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.96 & -3.94 \\ 0 & 7.89 \end{pmatrix}$	$\begin{pmatrix} 1.82 & -0.73 \\ -0.73 & 8.79 \end{pmatrix}$	21.82

TABLE III. Transformations used to construct C(100)/metal interface supercells.

Diamond	Metal	Transformation on Diamond lattice			Transformation on Metal lattice		
		T	S	Rotation (°)	T	S	Rotation (°)
C(110)	W	$\begin{pmatrix} 4.12 & 0 \\ 0 & 4.12 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.78 & 1.89 \\ 0 & 5.66 \end{pmatrix}$	$\begin{pmatrix} 3.70 & 0.74 \\ 0.74 & 5.92 \end{pmatrix}$	-11.31
	Cr	$\begin{pmatrix} 2.46 & 0 \\ 0 & 4.91 \end{pmatrix}$	–	0	$\begin{pmatrix} 2.50 & 2.50 \\ 0 & 7.50 \end{pmatrix}$	$\begin{pmatrix} 2.43 & 0.61 \\ 0.61 & 7.88 \end{pmatrix}$	-14.04
	Mo	$\begin{pmatrix} 4.12 & 0 \\ 0 & 4.12 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.81 & 1.90 \\ 0 & 5.71 \end{pmatrix}$	$\begin{pmatrix} 3.73 & 0.75 \\ 0.75 & 5.97 \end{pmatrix}$	-11.31
	Fe	$\begin{pmatrix} 2.45 & 0.82 \\ 0 & 3.27 \end{pmatrix}$	$\begin{pmatrix} 2.42 & 0.35 \\ 0.35 & 3.35 \end{pmatrix}$	-8.13	$\begin{pmatrix} 2.52 & 2.42 \\ 0 & 5.05 \end{pmatrix}$	$\begin{pmatrix} 2.39 & 0.80 \\ 0.80 & 5.59 \end{pmatrix}$	-18.43
	V	$\begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.95 & 1.95 \\ 0 & 5.84 \end{pmatrix}$	$\begin{pmatrix} 1.89 & 0.47 \\ 0.47 & 6.13 \end{pmatrix}$	-14.04
	Ir	$\begin{pmatrix} 2.83 & 0 \\ 0 & 3.54 \end{pmatrix}$	–	0	$\begin{pmatrix} 2.61 & -2.66 \\ 0 & 5.33 \end{pmatrix}$	$\begin{pmatrix} 2.47 & -0.83 \\ -0.83 & 5.90 \end{pmatrix}$	18.55
	Rh	$\begin{pmatrix} 2.83 & 0 \\ 0 & 3.54 \end{pmatrix}$	–	0	$\begin{pmatrix} 2.64 & -2.69 \\ 0 & 5.39 \end{pmatrix}$	$\begin{pmatrix} 2.50 & -0.84 \\ -0.84 & 5.96 \end{pmatrix}$	18.55
	Ti	$\begin{pmatrix} 2 & 0 \\ 0 & 5 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & -3.51 \\ 0 & 7.03 \end{pmatrix}$	$\begin{pmatrix} 1.60 & -0.64 \\ -0.64 & 7.83 \end{pmatrix}$	21.88
	Pt	$\begin{pmatrix} 4 & 0 \\ 0 & 4.95 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.60 & -3.64 \\ 0 & 7.28 \end{pmatrix}$	$\begin{pmatrix} 3.42 & -1.14 \\ -1.14 & 8.06 \end{pmatrix}$	18.49
	Cu	$\begin{pmatrix} 1 & 0 \\ 0 & 5 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.98 & -4.01 \\ 0 & 8.03 \end{pmatrix}$	$\begin{pmatrix} 0.90 & -0.4 \\ -0.4 & 8.97 \end{pmatrix}$	24.01
	Al	$\begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1.94 & 0.49 \\ 0.49 & 2.18 \end{pmatrix}$	-14.04	$\begin{pmatrix} 1.77 & -0.56 \\ 0 & 2.88 \end{pmatrix}$	$\begin{pmatrix} 1.75 & -0.21 \\ -0.21 & 2.93 \end{pmatrix}$	6.85
	Ag	$\begin{pmatrix} 2 & 0 \\ 0 & 5 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & -3.52 \\ 0 & 7.03 \end{pmatrix}$	$\begin{pmatrix} 1.60 & -0.64 \\ -0.64 & 7.83 \end{pmatrix}$	21.88
	Au	$\begin{pmatrix} 2 & 0 \\ 0 & 5 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & -3.51 \\ 0 & 7.01 \end{pmatrix}$	$\begin{pmatrix} 1.59 & -0.64 \\ -0.64 & 7.82 \end{pmatrix}$	21.88
	Mg	$\begin{pmatrix} 5.04 & 1.95 \\ 0 & 3.94 \end{pmatrix}$	$\begin{pmatrix} 4.93 & 1.07 \\ 0 & 4.27 \end{pmatrix}$	-12.26	$\begin{pmatrix} 3.97 & -1 \\ 0 & 5.07 \end{pmatrix}$	$\begin{pmatrix} 3.94 & -0.44 \\ -0.44 & 5.15 \end{pmatrix}$	6.30
	Zn	$\begin{pmatrix} 1.02 & 0 \\ 0 & 5.05 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.98 & -3.96 \\ 0 & 7.93 \end{pmatrix}$	$\begin{pmatrix} 0.90 & -0.40 \\ -0.40 & 8.86 \end{pmatrix}$	23.99

TABLE IV. Transformations used to construct C(110)/metal interface supercells.

4. Radial distribution function of C(100), C(110), C(111) and metals

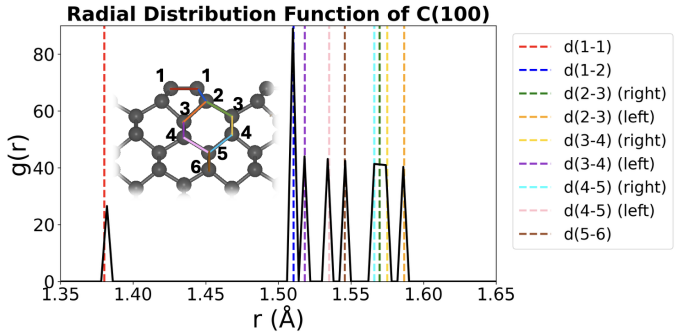
For diamond terminations exposing surface sp^2 bonds, comparing the radial distribution function $g(r)$ of the pristine surface with that of the same slab in the interfacial geometry provides a quantitative estimate of the fraction of sp^2

Diamond	Metal	Transformation on Diamond lattice			Transformation on Metal lattice		
		T	S	Rotation (°)	T	S	Rotation (°)
C(111)	W	$\begin{pmatrix} 3.61 & -3.61 \\ 0 & 7.21 \end{pmatrix}$	$\begin{pmatrix} 3.42 & -1.14 \\ -1.14 & 7.98 \end{pmatrix}$	18.43	$\begin{pmatrix} 3.30 & 2.02 \\ 0 & 6.06 \end{pmatrix}$	$\begin{pmatrix} 3.23 & 0.70 \\ 0.70 & 6.36 \end{pmatrix}$	-12.18
	Cr	$\begin{pmatrix} 1 & -8 \\ 0 & 16 \end{pmatrix}$	$\begin{pmatrix} 0.90 & -0.43 \\ -0.43 & 17.88 \end{pmatrix}$	25.20	$\begin{pmatrix} 1.02 & 4.99 \\ 0 & 14.96 \end{pmatrix}$	$\begin{pmatrix} 0.97 & 0.30 \\ 0.30 & 15.76 \end{pmatrix}$	-17.33
	Mo	$\begin{pmatrix} 3.61 & -3.61 \\ 0 & 7.21 \end{pmatrix}$	$\begin{pmatrix} 3.42 & -1.14 \\ -1.14 & 7.98 \end{pmatrix}$	18.43	$\begin{pmatrix} 3.33 & 2.04 \\ 0 & 6.12 \end{pmatrix}$	$\begin{pmatrix} 3.53 & 0.70 \\ 0.70 & 6.41 \end{pmatrix}$	-12.18
	Fe	$\begin{pmatrix} 3.61 & -1.94 \\ 0 & 4.16 \end{pmatrix}$	$\begin{pmatrix} 3.50 & -0.87 \\ -0.87 & 4.51 \end{pmatrix}$	14.04	$\begin{pmatrix} 3.72 & 1.46 \\ 0 & 3.94 \end{pmatrix}$	$\begin{pmatrix} 3.65 & 0.69 \\ 0.69 & 4.14 \end{pmatrix}$	-10.77
	V	$\begin{pmatrix} 1.01 & -5.02 \\ 0 & 10.04 \end{pmatrix}$	$\begin{pmatrix} 0.92 & -0.42 \\ -0.42 & 11.21 \end{pmatrix}$	24.42	$\begin{pmatrix} 0.99 & 2.99 \\ 0 & 8.97 \end{pmatrix}$	$\begin{pmatrix} 0.94 & 0.28 \\ 0.28 & 9.45 \end{pmatrix}$	-16.72
	Ir	$\begin{pmatrix} 4.36 & 0 \\ 0 & 4.36 \end{pmatrix}$	–	0	$\begin{pmatrix} 4.02 & 0 \\ 0 & 4.02 \end{pmatrix}$	–	0
	Rh	$\begin{pmatrix} 4.36 & 0 \\ 0 & 4.36 \end{pmatrix}$	–	0	$\begin{pmatrix} 4.07 & 0 \\ 0 & 4.07 \end{pmatrix}$	–	0
	Ti	$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & 0 \\ 0 & 1.72 \end{pmatrix}$	–	0
	Pt	$\begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.60 & 0 \\ 0 & 3.60 \end{pmatrix}$	–	0
	Cu	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	–	0	$\begin{pmatrix} 0.98 & 0 \\ 0 & 0.98 \end{pmatrix}$	–	0
	Al	$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.77 & 0 \\ 0 & 1.77 \end{pmatrix}$	–	0
	Ag	$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & 0 \\ 0 & 1.72 \end{pmatrix}$	–	0
	Au	$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$	–	0	$\begin{pmatrix} 1.72 & 0 \\ 0 & 1.72 \end{pmatrix}$	–	0
	Mg	$\begin{pmatrix} 4.36 & 0 \\ 0 & 4.36 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.43 & 0 \\ 0 & 3.43 \end{pmatrix}$	–	0
	Zn	$\begin{pmatrix} 3.61 & 0 \\ 0 & 3.61 \end{pmatrix}$	–	0	$\begin{pmatrix} 3.47 & 0 \\ 0 & 3.47 \end{pmatrix}$	–	0

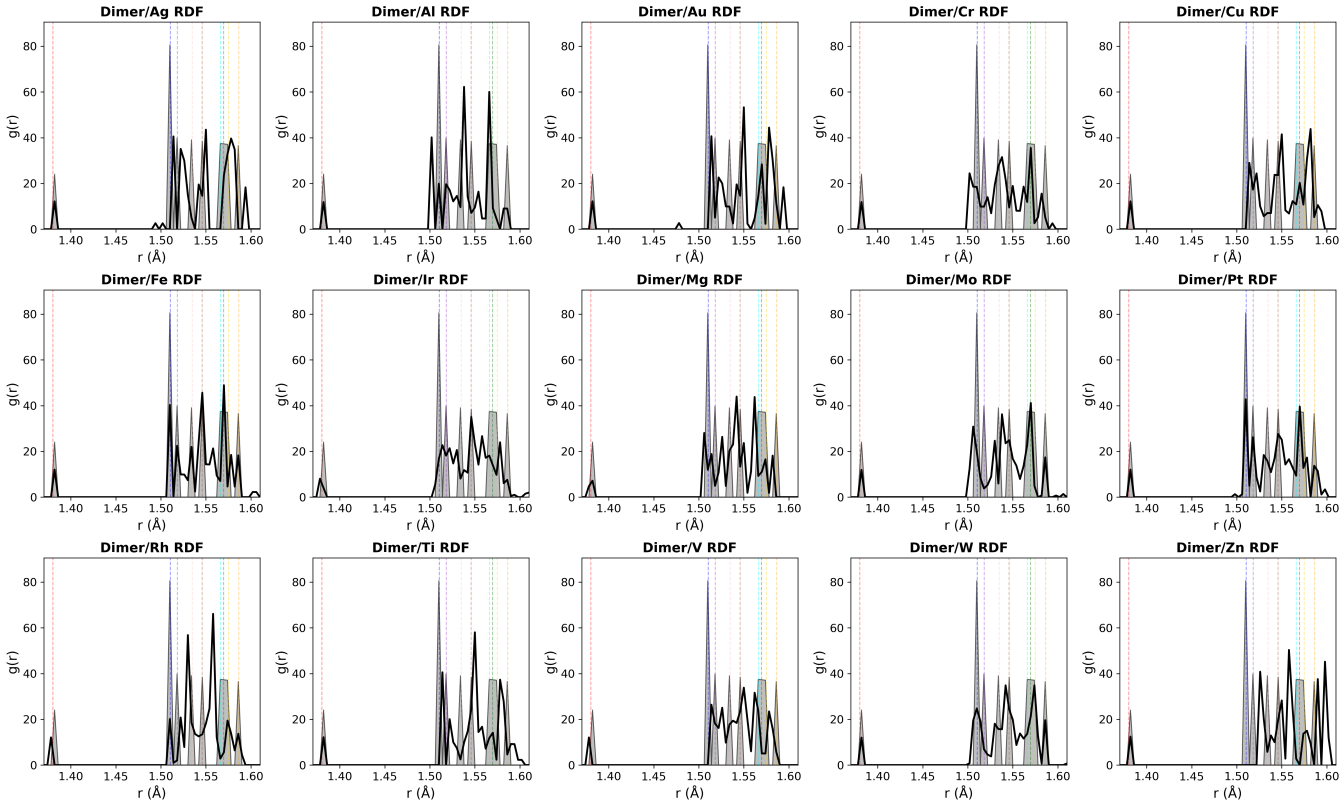
TABLE V. Transformations used to construct C(111)/metal interface supercells.

bonds preserved upon contact (see main text). For completeness, in Fig.2 and 3 we report the corresponding $g(r)$ analysis for C(100) and C(110); a more detailed discussion is given in the main text.

For the unreconstructed C(111) surface, a reconstruction upon contact is not expected; rather, the dominant interfacial response is the saturation of its reactive dangling bonds via C-metal bond formation. Nevertheless, $g(r)$ remains a convenient monitor of the structural changes induced by interface formation, both for this diamond termination and for the metallic slabs. We report the $g(r)$ analysis in Fig.4 for C(111) and in Fig.5, 6, 7, 8 for all metals. For C(111), in most cases the peak associated with the sp^3 C-C bond within the surface bilayer is only reduced in intensity and slightly broadened. More pronounced perturbations are observed for interfaces with Cr, Ti and V, which also correspond to the highest adhesion energy values with this diamond termination. For the metals, since the slabs are subject to strain, the reference $g(r)$ is computed for the isolated metal slab within the same interface cell. A qualitative comparison shows that the largest peak perturbations occur for transition metals such as V, Ti, Mo and Cr, consistently with their stronger adhesion across all diamond terminations.

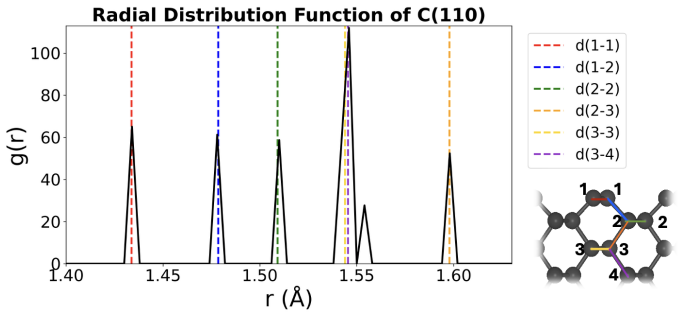


(a)

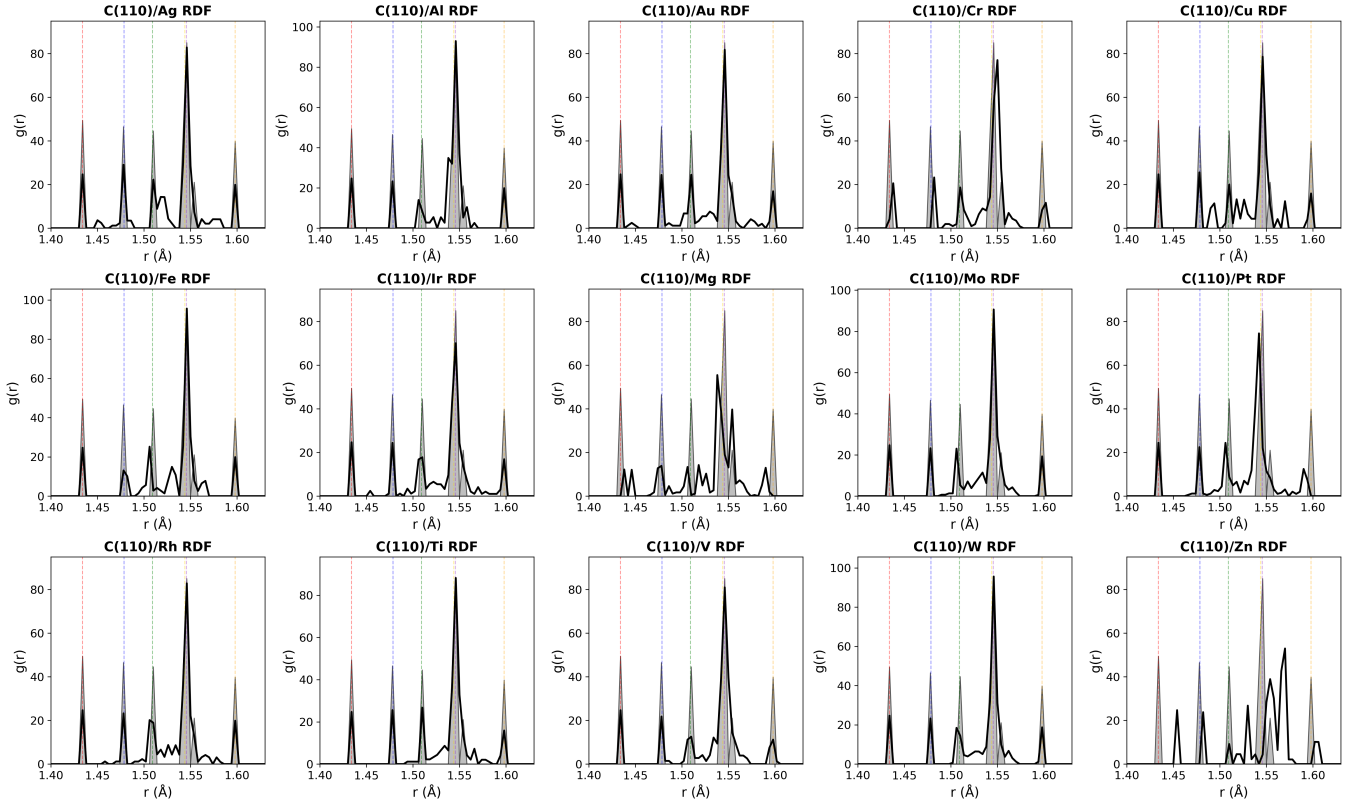


(b)

FIG. 2. (a) Radial distribution function of pristine C(100). Coloured dashed lines identify peaks corresponding to the interatomic distances highlighted in the schematic. (b) Radial distribution function of C(100) in the optimized interface geometry (black line), compared with the $g(r)$ of the pristine surface (plotted in the background with faded lines).

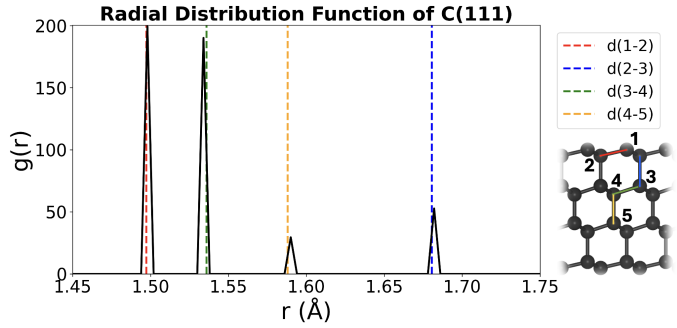


(a)

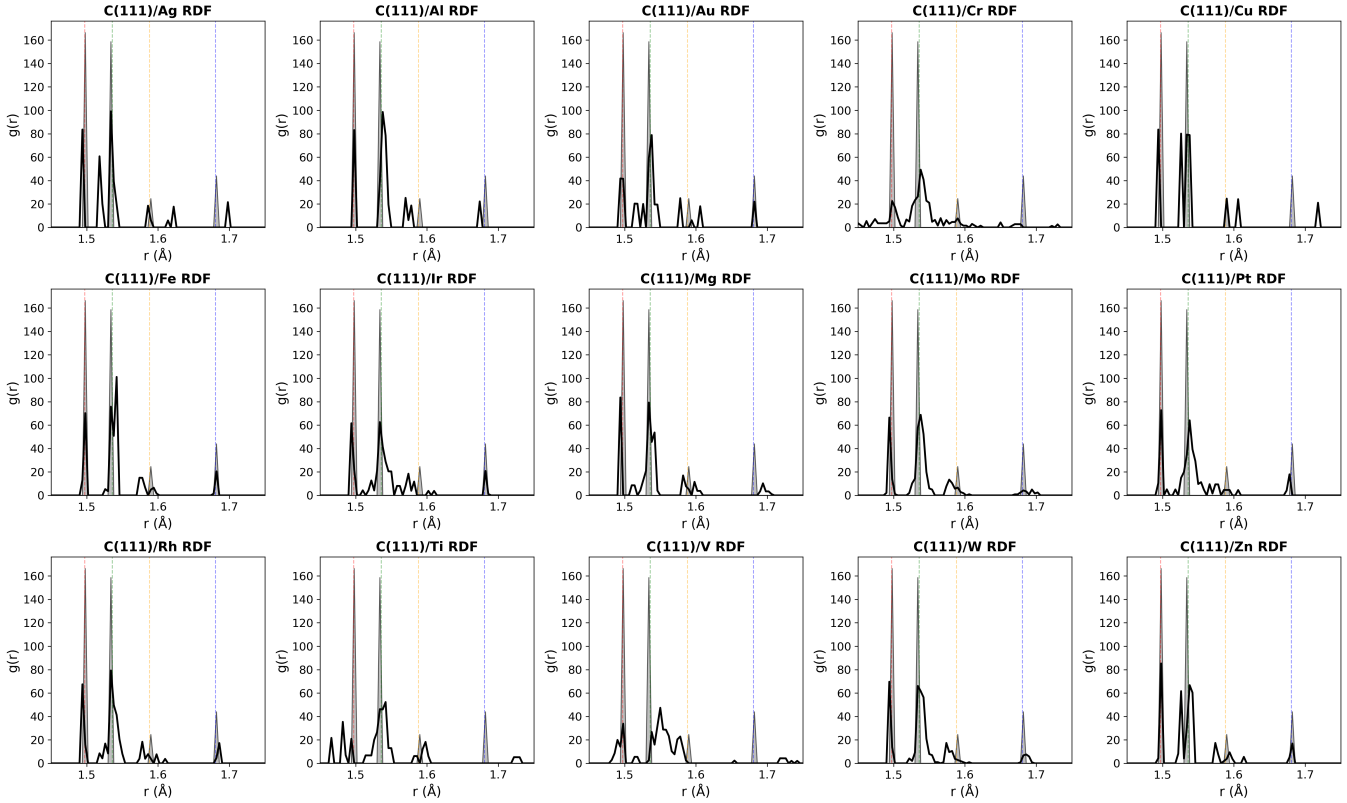


(b)

FIG. 3. (a) Radial distribution function of pristine C(110). Coloured dashed lines identify peaks corresponding to the interatomic distances highlighted in the schematic. (b) Radial distribution function of C(110) in the optimized interface geometry (black line), compared with the $g(r)$ of the pristine surface (plotted in the background with faded lines).

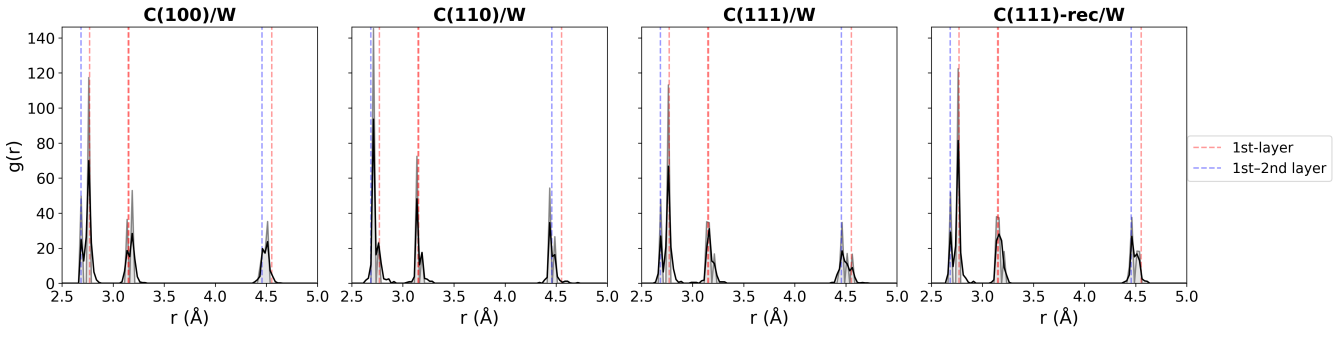


(a)

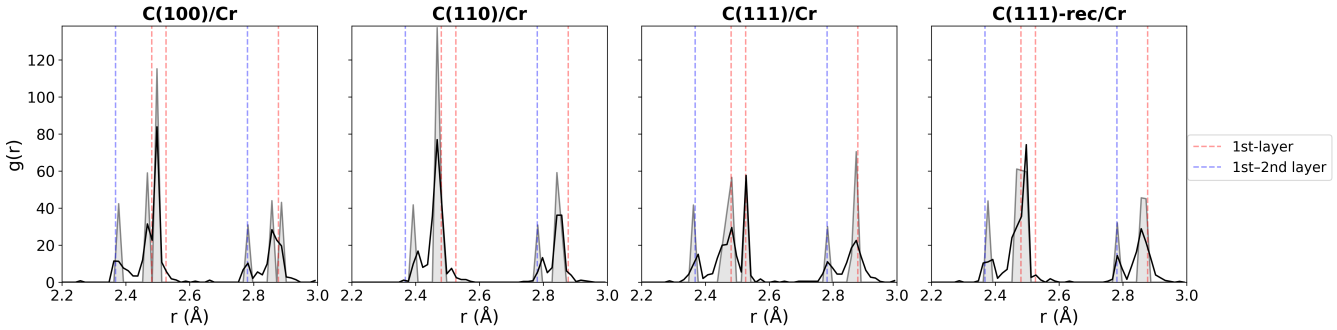


(b)

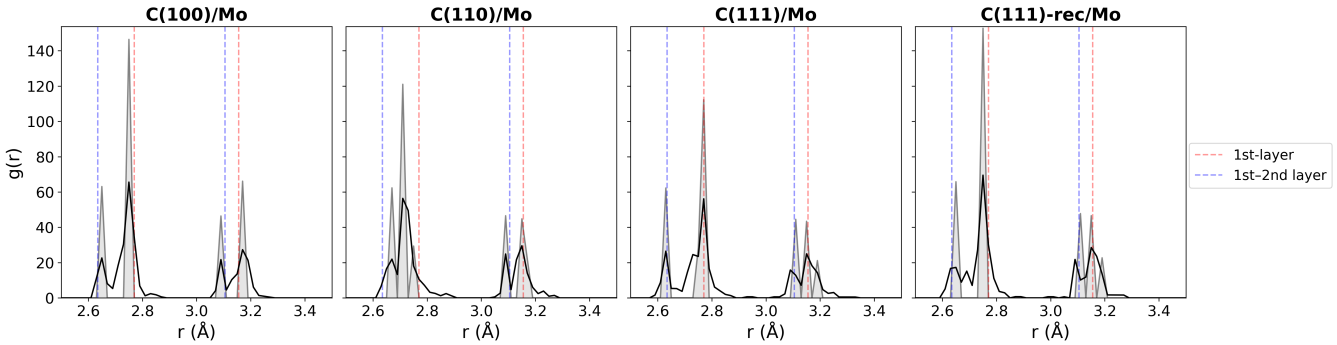
FIG. 4. (a) Radial distribution function of pristine C(111). Coloured dashed lines identify peaks corresponding to the interatomic distances highlighted in the schematic. (b) Radial distribution function of C(111) in the optimized interface geometry (black line), compared with the $g(r)$ of the pristine surface (plotted in the background with faded lines).



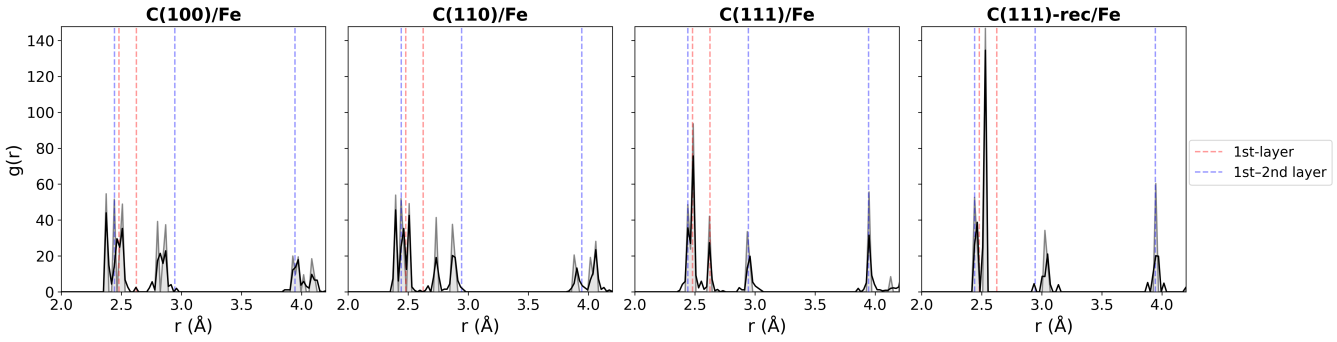
(a)



(b)

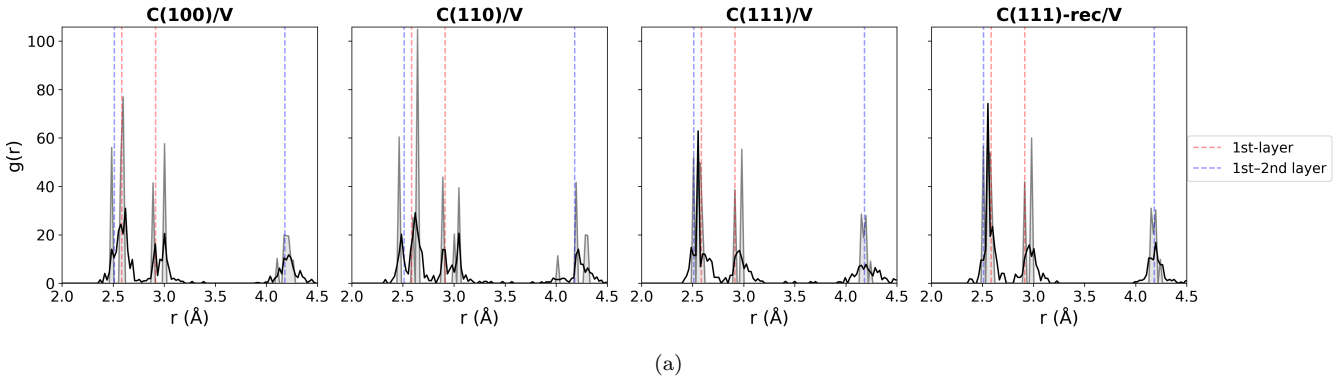


(c)

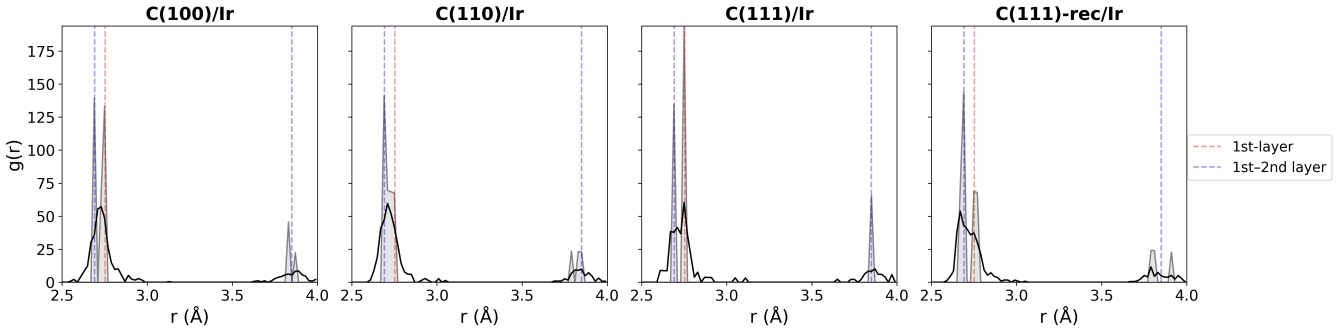


(d)

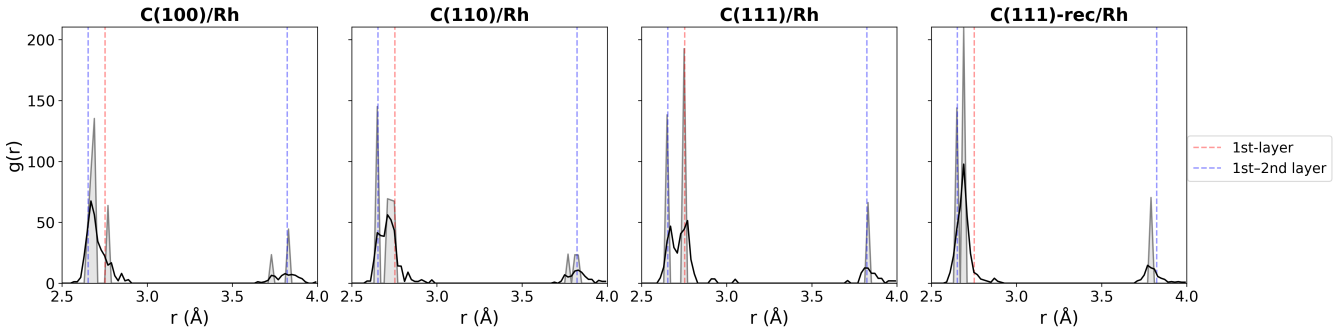
FIG. 5. Radial distribution function $g(r)$ of the metal slab in the optimized interface geometry (black line), compared with the $g(r)$ of the corresponding pristine metal slab (grey, faded), for interfaces between the metal and the four diamond terminations (C(100), C(110), C(111), and C(111)-rec). Each panel reports the results for a different metal: (a) W, (b) Cr, (c) Mo, (d) Fe. Coloured dashed lines indicate reference interatomic distances within the first metal layer (red) and between the first and second metal layers (blue).



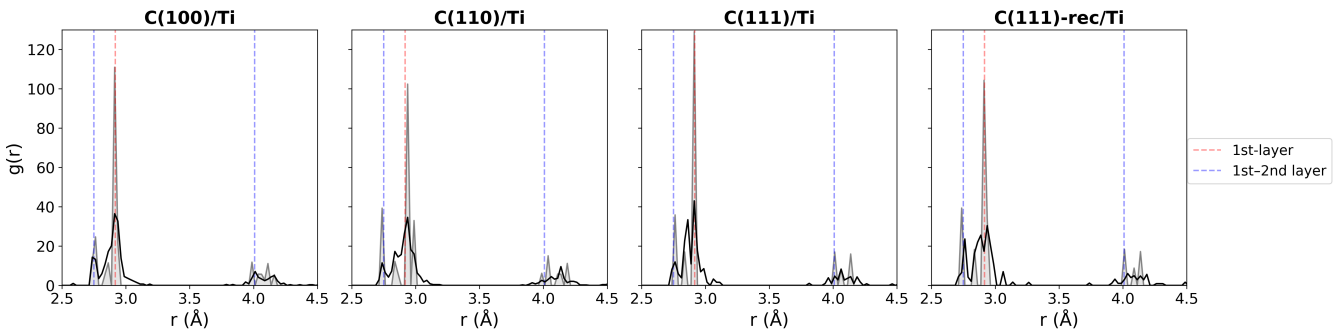
(a)



(b)

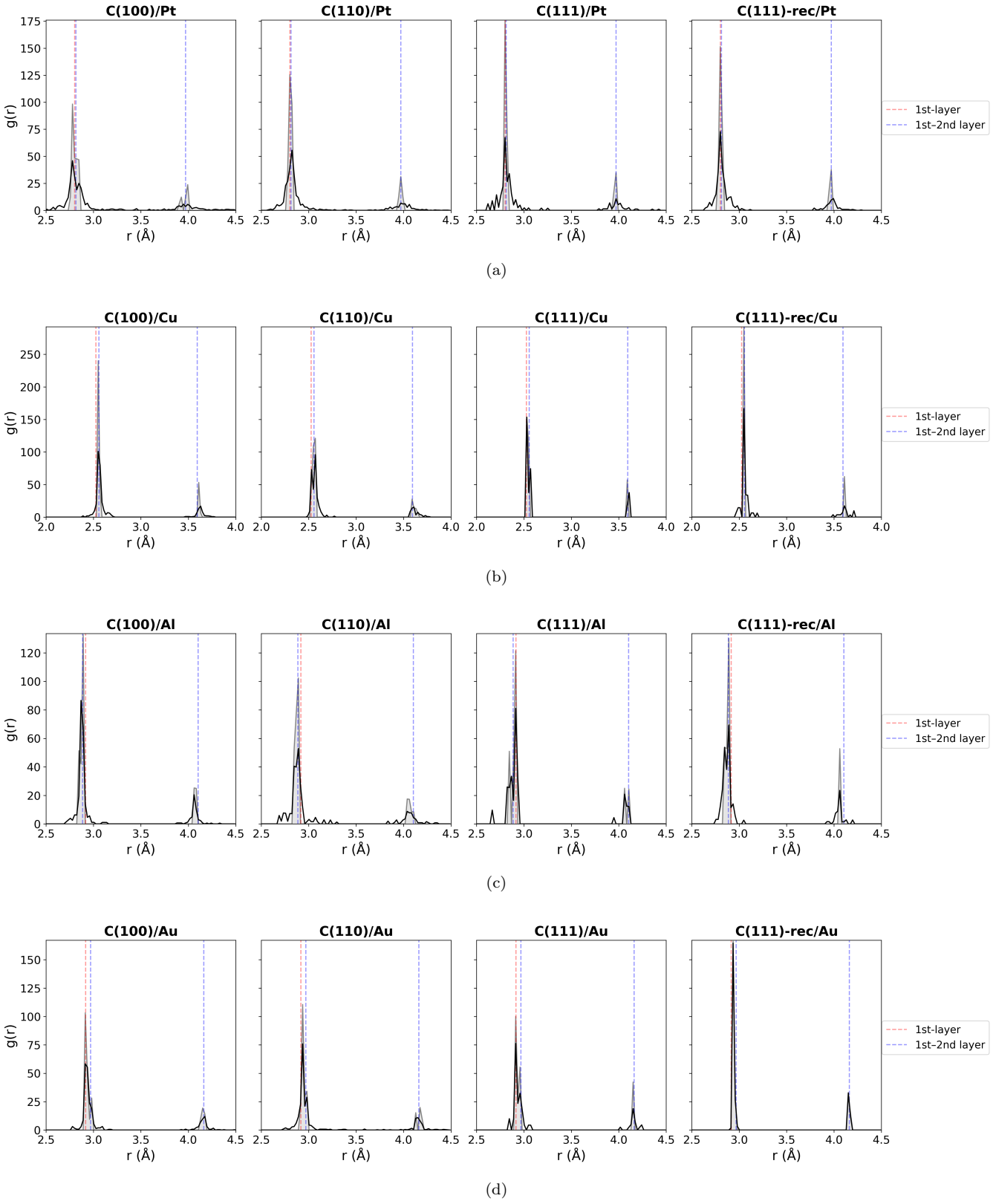


(c)



(d)

FIG. 6. (Radial distribution function $g(r)$ of the metal slab in the optimized interface geometry (black line), compared with the $g(r)$ of the corresponding pristine metal slab (grey, faded), for interfaces between the metal and the four diamond terminations (C(100), C(110), C(111), and C(111)-rec). Each panel reports the results for a different metal: (a) V, (b) Ir, (c) Rh, (d) Ti. Coloured dashed lines indicate reference interatomic distances within the first metal layer (red) and between the first and second metal layers (blue).



(a)

(b)

(c)

(d)

FIG. 7. Radial distribution function $g(r)$ of the metal slab in the optimized interface geometry (black line), compared with the $g(r)$ of the corresponding pristine metal slab (grey, faded), for interfaces between the metal and the four diamond terminations (C(100), C(110), C(111), and C(111)-rec). Each panel reports the results for a different metal: (a) Pt, (b) Cu, (c) Al, (d) Au. Coloured dashed lines indicate reference interatomic distances within the first metal layer (red) and between the first and second metal layers (blue).

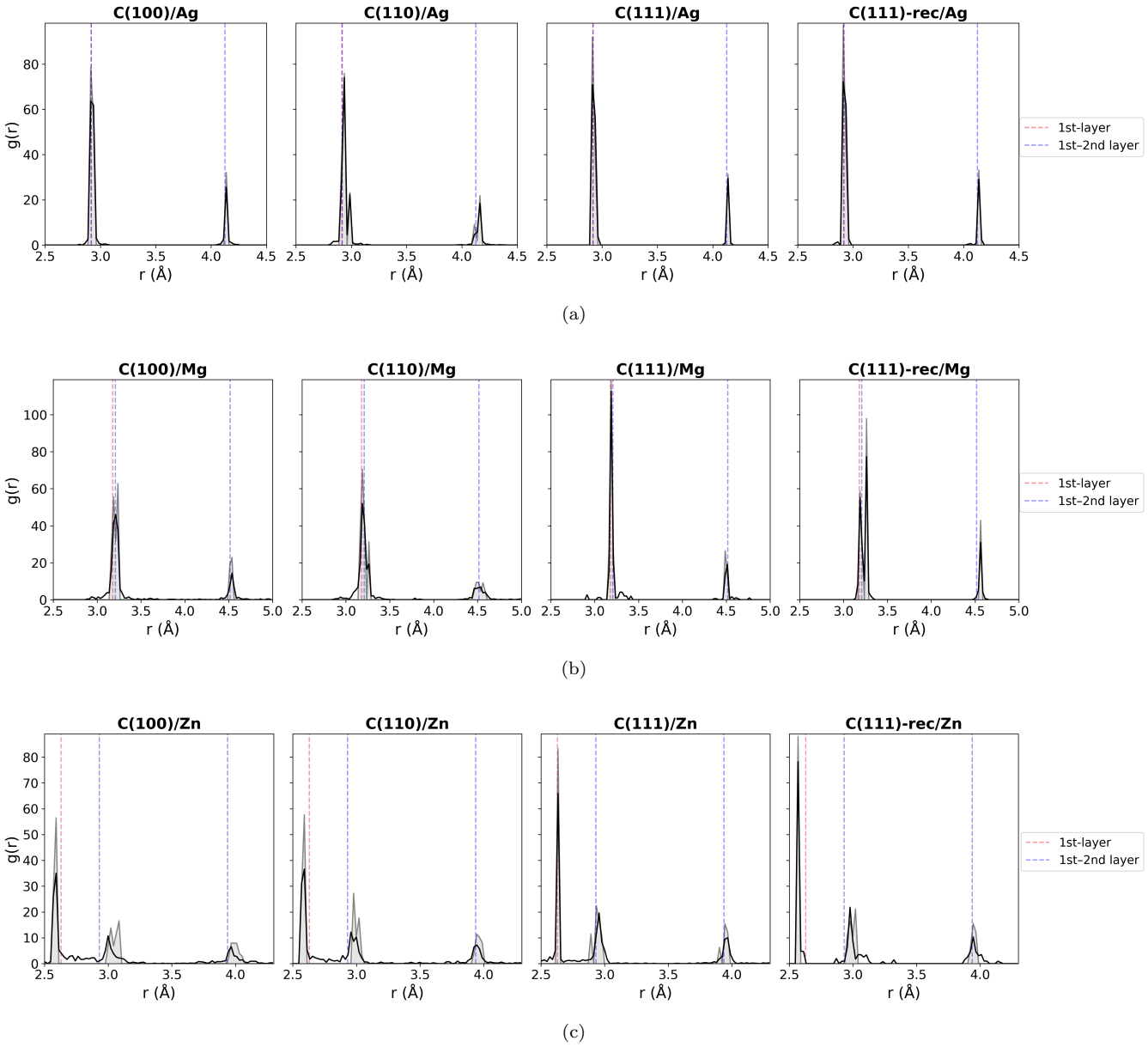


FIG. 8. Radial distribution function $g(r)$ of the metal slab in the optimized interface geometry (black line), compared with the $g(r)$ of the corresponding pristine metal slab (grey, faded), for interfaces between the metal and the four diamond terminations (C(100), C(110), C(111), and C(111)-rec). Each panel reports the results for a different metal: (a) Ag, (b) Mg, (c) Zn. Coloured dashed lines indicate reference interatomic distances within the first metal layer (red) and between the first and second metal layers (blue).