Supporting Information

Prediction of a New BeC Monolayer with Perfectly Planar Tetracoordinate Carbons†

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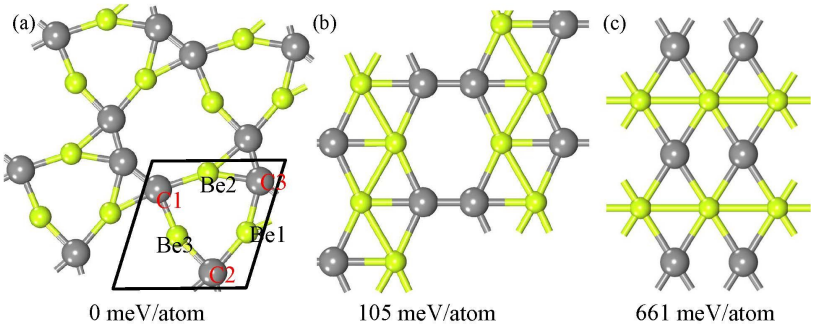
Figure S1. Top view of the BeC monolayer and other lying isomers found by the particle swarm search. Optimized coordinates of the unit cell for the lowest-energy structure with a=b=4.35 Å, c=20 Å, α =β=90° and γ=83.15°. The green and grey balls represent Be and C atoms.



atom	*x*	*y*	*z*
Be	0.336607	0.336607	0.5
Be	0.237067	0.850657	0.5
Be	0.850657	0.237067	0.5
C	0.856937	0.856937	0.5
C	0.0185469	0.561707	0.5
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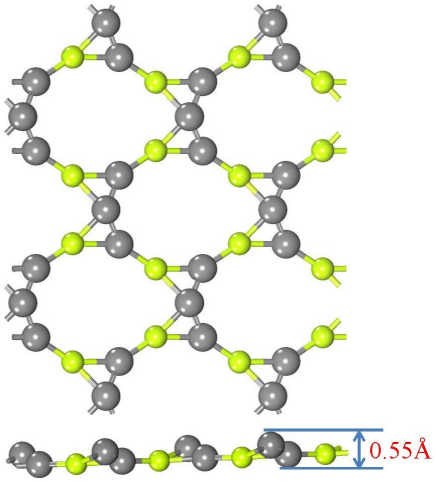
TableS1. The Hirshfeld Charge analysis of the BeC monolayer.

atoms	*Hirshfeld Charge(e)*
Be1	0.18
Be2	0.18
Be3	0.20
C1	-0.25
C2	-0.25
C3	-0.06

	Bond	Overlap Population
Covalent bond	C1-C3	1.15
	C2-C3	1.15
	Be3-C2	0.78
	Be3-C1	0.78
Partially covalent/ionic bond	Be2-C1	0.52
	Be1-C2	0.52
Ionic bond	Be2-C2	0.05
	Be1-C1	0.05
	Be1-C3	0.13
	Be2-C3	0.13

TableS2. The overlap population analysis of BeC.

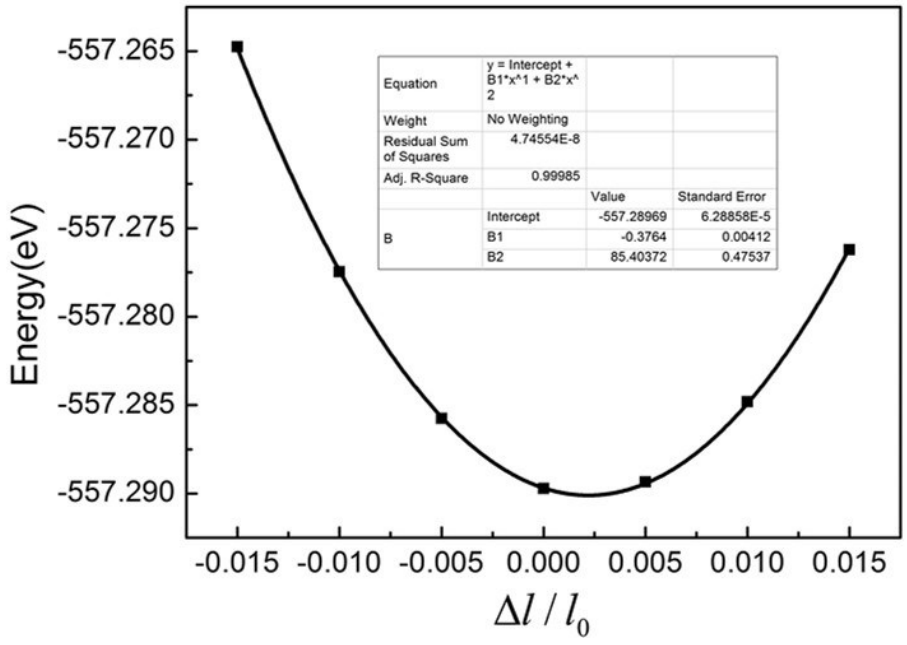
Figure S2. The optimized structure of the BeC monolayer with the Be_3 atom deficient in the primitive cell. The green and grey balls represent Be and C atoms.



In-plane stiffness calculation method

The in-plane stiffness(C) is defined as $C = \left[\partial E / \partial \delta^2 \right] / S_0$, in which E is the total energy, δ stands for the applied uniaxial strain and S_0 is the area of the optimized structure. To compute the in-plane stiffness(C) , we dilate the lattice of the cell up to 1.5% and the total energy – deformation is shown in FigureS3.

Figure S3. Strain-total energy relations of the BeC monolayer. $\Delta l/l_0$ is the dilation of the lattice constant.



Carrier mobility calculation method

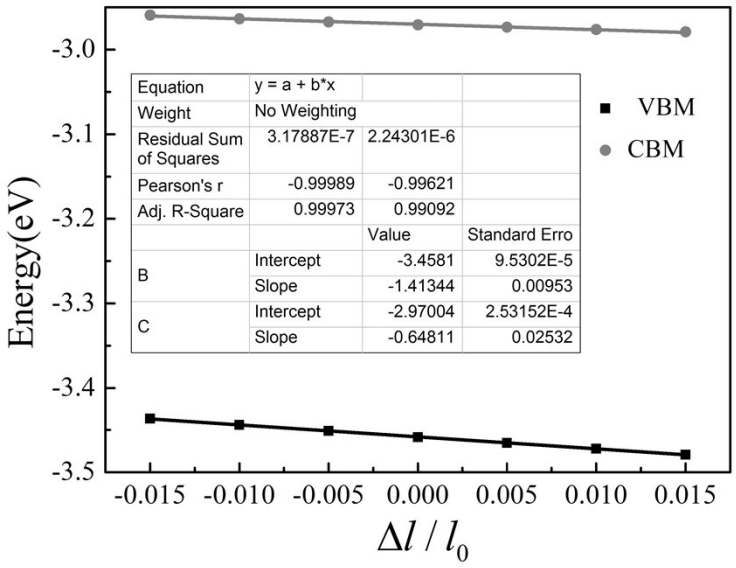
The acoustic-phonon-limited carrier mobility (μ) in 2D materials under effective mass approximation can be expresses as:[1-4]

$$\mu = \frac{2e\hbar^3 C}{3k_B T \left| m^* \right|^2 E_1^2} \qquad (2)$$

Here, T is the temperature (set at 300K), C is the elastic modulus (in-plane stiffness) and m* is the effective mass. The deformation potential constant E_1 is derived from $\Delta E = E_1 (\Delta l/l_0)$, in which ΔE is the energy shift of band edge with respect to lattice

dilation ($\Delta l/l_0$). The positions of VBM and CBM with respect to the strain are plotted in Figure S4.

Figure S4. Shifts of VBM and CBM under uniaxial strains for monolayer BeC. $\Delta l/l_0$ is the dilation of lattice constant. The vacuum level is set at 0 for reference.



Reference:

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2. M. Q. Long, L. Tang, D. Wang, L. Wang, Z. Shuai, *J. Am. Chem.Soc.*, 2009, **131**, 17728-17729.

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