Colossal band gap response of single-layer phosphorene to strain predicted by Quantum Monte Carlo

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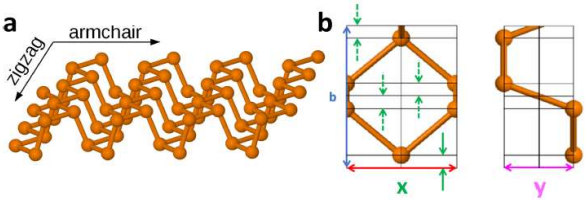
1.Introduction

Two-dimensional (2D) materials have the potential to revolutionize technology. However, the band gaps of 2D materials under strain still cannot be predicted accurately.

By using ultra-accurate quantum Monte Carlo methods, we predict that single-layer phosphorene is not only exhibits a band gap straining rate 0.1eV/% but it keeps the direct Γ → Γ transition over a very large window of applied strains.

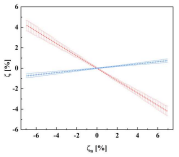


2. Optimization of Structure

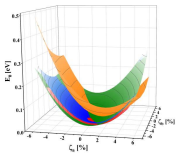
Four dimensional paraboloid approximation is applied to fit potential energy surface and get minima.

parameter	QMC 11-cell	QMC 16-cell	QMC 22-cell	QMC 32-cell	DFT-PBE	3D-BP
	ground state					
a	6.229±0.008	6.238±0.002	6.230±0.002	6.236±0.003	6.235	6.2618
b	8.651±0.017	8.688±0.008	8.707±0.006	8.704±0.011	8.711	8.2700
x	0.748±0.005	0.759±0.002	0.765±0.001	NA	0.770	0.6367
y	3.987±0.007	3.978±0.003	3.985±0.002	NA	3.975	4.0280
E_0^s	-716.563±0.002	-716.498±0.0008	-716.469±0.0007	-716.453±0.001	-717.711	NA
	excited state					
a	6.227±0.027	6.222±0.003	6.224±0.003	6.235±0.003	6.222	NA
b	8.515±0.178	8.607±0.012	8.664±0.010	8.640±0.014	8.543	NA
x	0.728±0.044	0.747±0.003	0.761±0.002	NA	0.739	NA
y	4.053±0.018	4.031±0.002	4.020±0.002	NA	4.051	NA
E_1^s	-716.415±0.005	-716.375±0.0007	-716.375±0.001	-716.378±0.001	-717.643	NA

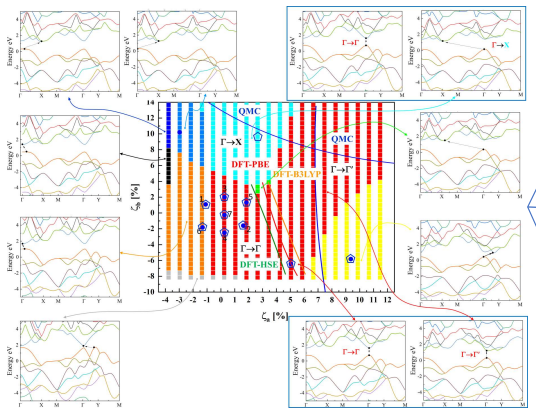
Negative Poisson ratio



Deformation energy



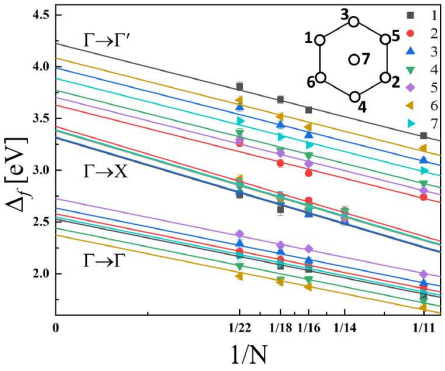
3.Outline of DFT phase diagram and finite size effect



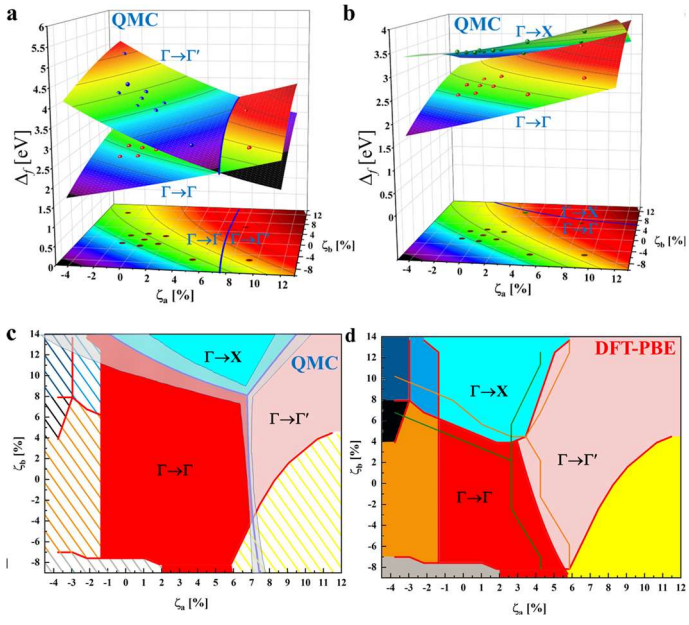
Γ → Γ'

Γ → X

Γ → Γ



4. Conclusions



1. The Γ → Γ QMC band gap may have a significantly wider window.

2. For our QMC optimized structure at equilibrium we obtain
a = 3.30±0.003Å,
b = 4.61±0.006 Å
Δ_f = 2.53±0.020 eV (experiment 2.46 eV)

3. The band gap tuning rates is 0.1 eV/% strain. The direct band gap at Γ is in the range of 2.1 - 3.8 eV.