Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Polymorphs of Two Dimensional Phosphorus and Arsenic: an Insight from Evolutionary Search
Supplementary Information

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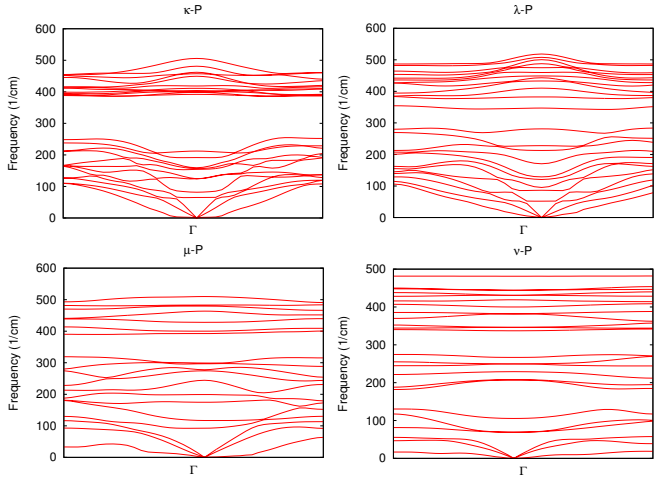

FIG. 1. Phonon dispersion of newly predicted monolayer phosphorus allotropes, shown along two high symmetry directions from Γ point.

Allotrope	GGA bandgap (eV)	HSE bandgap (eV)
κ-P	1.54	2.34
λ-P	1.21	1.84
μ-P	1.43	2.18
ν-P	1.71	2.60
κ-As	1.34	1.94
λ-As	0.83	1.46
μ-As	1.16	1.84
ν-As	1.12	1.76

TABLE I. GGA and HSE bandgap of newly discovered monolayer P and As allotropes.

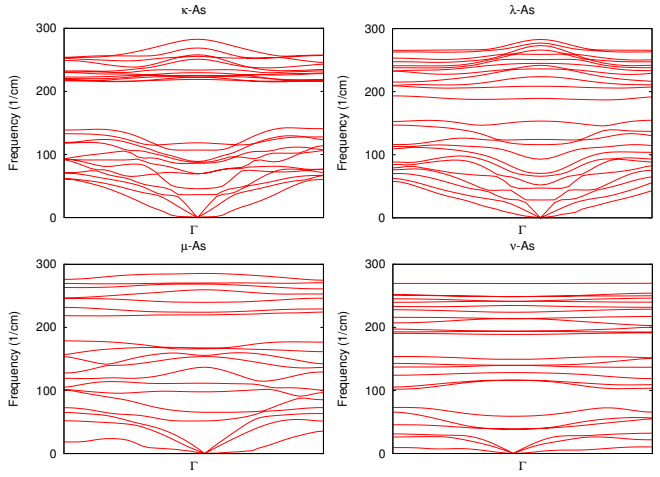

FIG. 2. Phonon dispersion of newly predicted monolayer arsenic allotropes, shown along two high symmetry directions from Γ point.

I. CRYSTAL STRUCTURE OF NEWLY PREDICTED MONOLAYER P ALLOTROPES

Atomic positions are given in terms of lattice vectors $\vec{a}, \vec{b}, \vec{c}$.

κ-P:
$\vec{a} = (9.7134, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 3.3011, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
P 0.1744 0.0000 0.5345
P 0.3256 0.0000 0.4655
P 0.4538 0.5000 0.5025
P 0.0462 0.5000 0.4975
P 0.6062 0.5000 0.4343
P 0.8938 0.5000 0.5657
P 0.7503 0.0000 0.4550
P 0.7497 0.0000 0.5450

λ-P:
$\vec{a} = (9.4213, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 3.2753, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
P 0.4245 0.5000 0.4047
P -0.0043 0.5000 0.4103
P 0.4195 0.5000 0.3149
P 0.7674 0.5000 0.3784
P 0.7812 0.0000 0.3174
P 0.5537 0.0000 0.2846
P 0.2760 0.0000 0.4258
P 0.1020 0.0000 0.3629

μ-P:
$\vec{a} = (7.2373, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 4.5891, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
As 0.8389 0.4259 0.3125
As 0.0677 0.7351 0.3299
As 0.5775 0.6714 0.3021
As 0.4006 0.2656 0.3204
As 0.7751 0.2606 0.3934
As 0.5458 0.9518 0.3757
As 1.0371 1.0151 0.4035
As 0.2141 0.4207 0.3847

ν-P:
$\vec{a} = (5.9500, 0.0000, 0.0000)$
$\vec{b} = (-2.975, 5.1529, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
P 0.6495 -0.0118 0.4985
P 0.5704 0.8538 0.4135
P 0.0118 0.6612 0.4985
P 0.1462 0.7166 0.4135
P 0.3388 0.3505 0.4985
P 0.2834 0.4296 0.4135
P 0.3333 0.6667 0.5433
P 0.0000 0.0000 0.5308

II. CRYSTAL STRUCTURE OF NEWLY PREDICTED MONOLAYER AS ALLOTROPES

Atomic positions are given in terms of lattice vectors $\vec{a}, \vec{b}, \vec{c}$.

κ-As:
$\vec{a} = (10.3246, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 3.6348, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
As 0.1722 0.0000 0.5384
As 0.3278 0.0000 0.4616
As 0.4603 0.5000 0.5039
As 0.0397 0.5000 0.4961
As 0.6113 0.5000 0.4259
As 0.8887 0.5000 0.5741
As 0.7649 0.0000 0.4511
As 0.7351 0.0000 0.5489

λ-As:
$\vec{a} = (9.9968, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 3.6070, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
As 0.4394 0.5000 0.4098
As 0.0009 0.5000 0.4142
As 0.4044 0.5000 0.3119
As 0.7607 0.5000 0.3806
As 0.7803 0.0000 0.3129
As 0.5456 0.0000 0.2750
As 0.2790 0.0000 0.4345
As 0.1097 0.0000 0.3602

μ-As:
$\vec{a} = (7.8819, 0.0000, 0.0000)$
$\vec{b} = (0.0000, 4.8449, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
As 0.8241 0.3699 0.3076
As 0.0509 0.7154 0.3277
As 0.5588 0.6324 0.2935
As 0.3684 0.2175 0.3147
As 0.7458 0.2439 0.3982
As 0.5190 0.8993 0.3776
As 1.0111 0.9804 0.4120
As 0.2013 0.3961 0.3908

ν-As:
$\vec{a} = (6.3500, 0.0000, 0.0000)$
$\vec{b} = (-3.175, 5.4993, 0.0000)$
$\vec{c} = (0.0000, 0.0000, 25.0000)$
ATOMIC POSITIONS
As 0.6542 0.0093 0.4996
As 0.5840 0.8557 0.4064
As -0.0093 0.6449 0.4996
As 0.1443 0.7283 0.4064
As 0.3551 0.3458 0.4996
As 0.2717 0.4160 0.4064
As 0.3333 0.6667 0.5498
As 0.0000 0.0000 0.5421