

Supplemental Material for: “Polaron-assisted electronic transport in ZnP₂ nanowires”

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S1. DENSITY FUNCTIONAL THEORY RESULTS

The spin-unpolarized local density of states (LDOS) for the pristine ZnP₂ in the monoclinic geometry is depicted in the Figure S1. In Figure S2 we show the effect of Hubbard correction on P-P and Zn-d states. Figure S3 represents the charged $1V_{Zn}1P_i$ -I calculations.

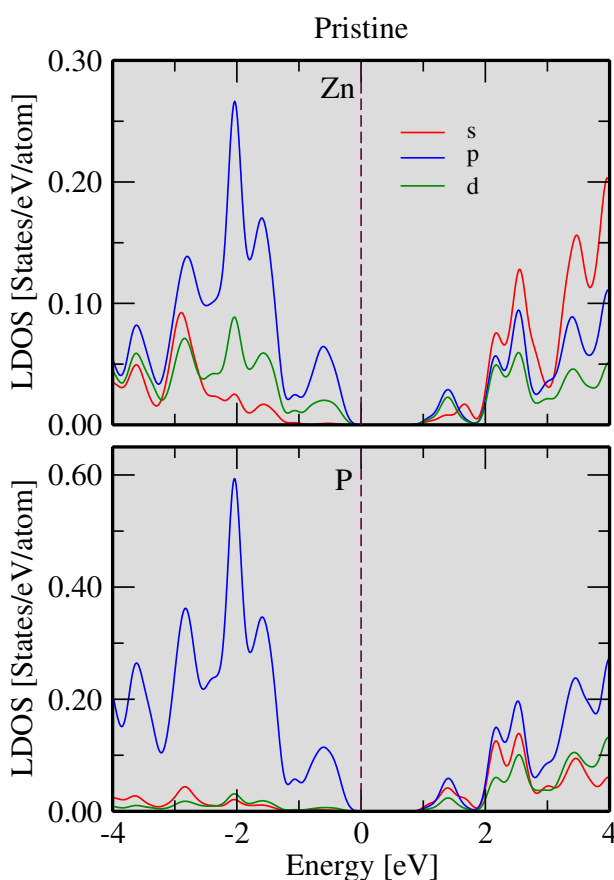


Figure S1. Calculated density of states for the pristine ZnP₂ using HSE06 XC. In upper panel is shown the Zn calculation, while the bottom part represent the P states investigation.

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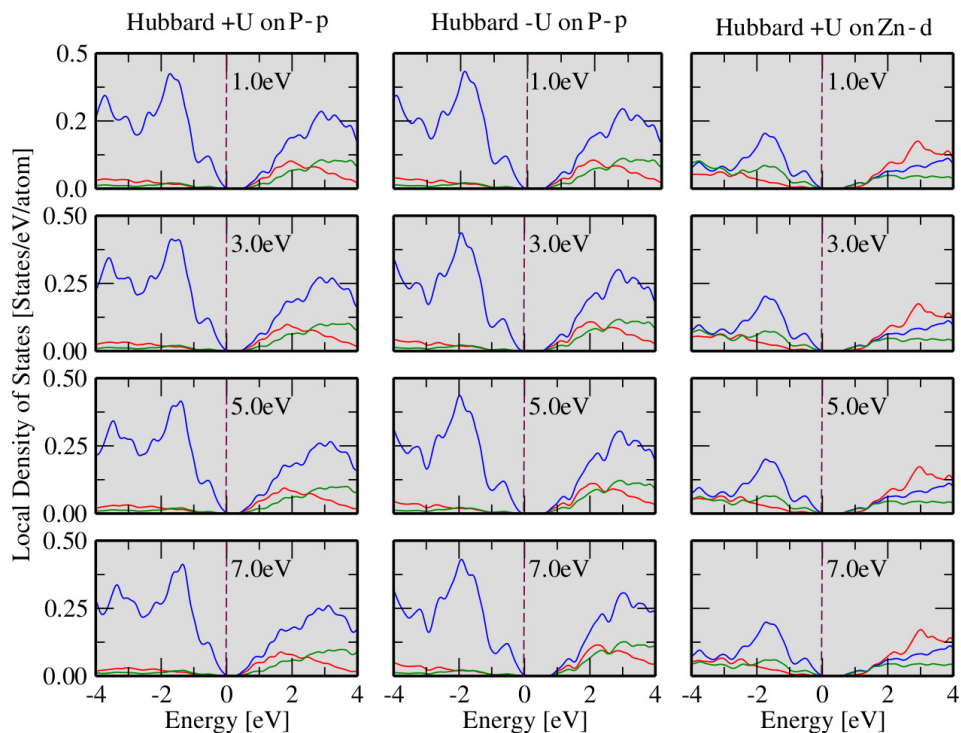


Figure S2. Calculated density of states using PBE Hubbard correction on P-*p* and Zn-*d* states.

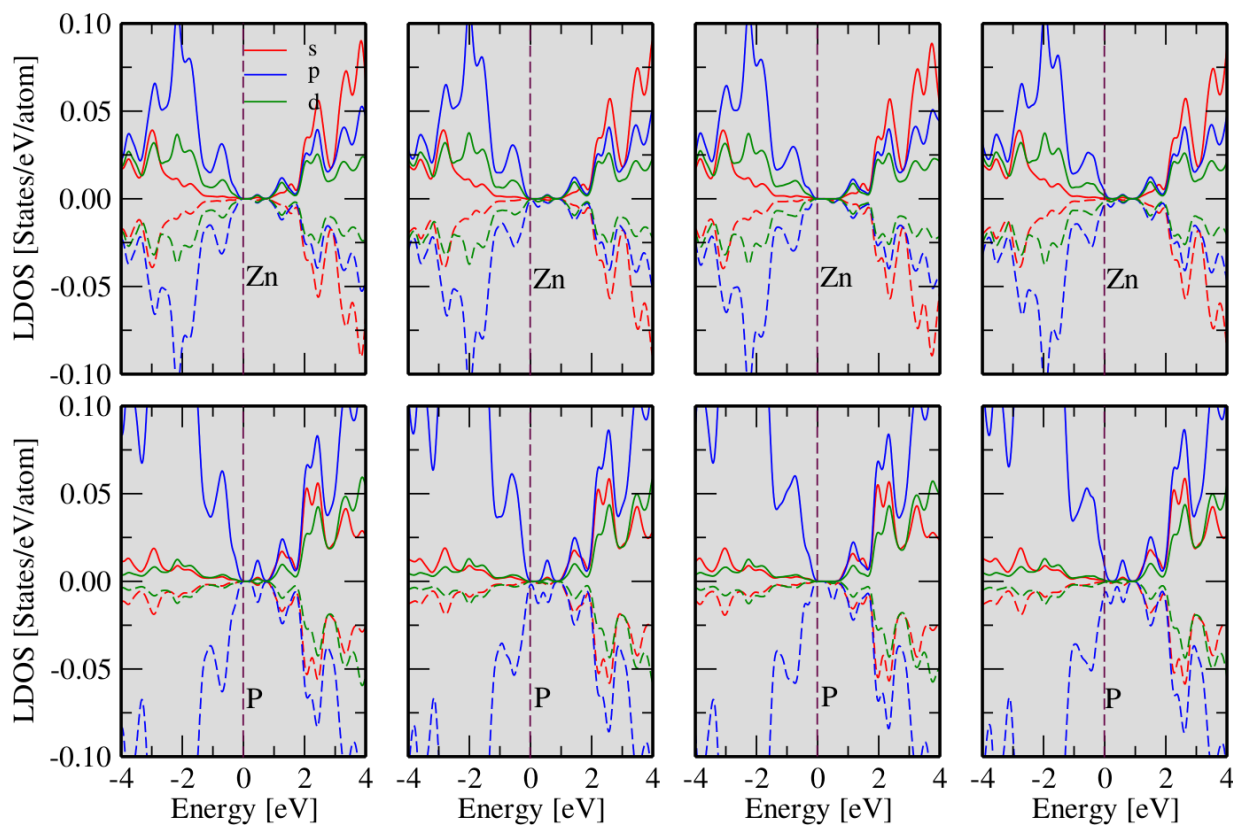


Figure S3. Calculated local density of states for the structure $1V_{Zn}1P_I-I$. From left to right panel columns, we have optimized the system with different charges $q = -1, +1, -2$ and $+2$, respectively. The upper and bottom panels show the zinc and phosphor local density of states, respectively.

S2. OPTIMIZED STRUCTURES

This section presents the lattice parameters and atomic positions of structures optimized with HSE06 XC.

A. $1V_{Zn}1P_i-I$

SYSTEM = ZnP2

1.0000000000000000

17.6369807634095999 0.0000000000000000 -0.0504105781290306
 0.0000000000000000 14.6753022059525247 0.0000000000000000
 -3.2408554168070340 0.0000000000000000 14.8647166764882588

Zn P

63 128

Direct

0.1972706152132154 0.0476302361951876 0.1106909501739330
 0.6957363092434580 0.0476646519952493 0.1120378083134670
 0.1969914349991735 0.5474669590703487 0.1119716859974273
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B. $1V_{Zn}1P_i$ -II

SYSTEM = ZnP2

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | \\ | |
| 17.6369807634095999 | 0.0000000000000000 | -0.0504105781290306 |
| 0.0000000000000000 | 14.6753022059525247 | 0.0000000000000000 |
| -3.2408554168070340 | 0.0000000000000000 | 14.8647166764882588 |

Zn P
63 129

Direct

| | | |
|--------------------|--------------------|--------------------|
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| 0.8033923809361809 | 0.7977603311642838 | 0.6374209048216173 |
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Zn P

62 129

Direct

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