

## Supporting Information

### Significant enhancement of the thermoelectric properties of CaP3 through reducing dimensionality

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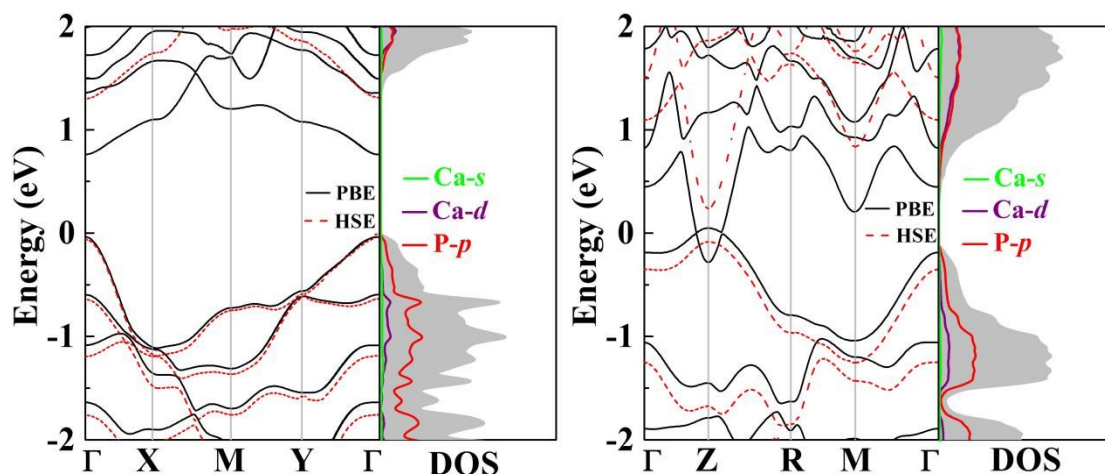
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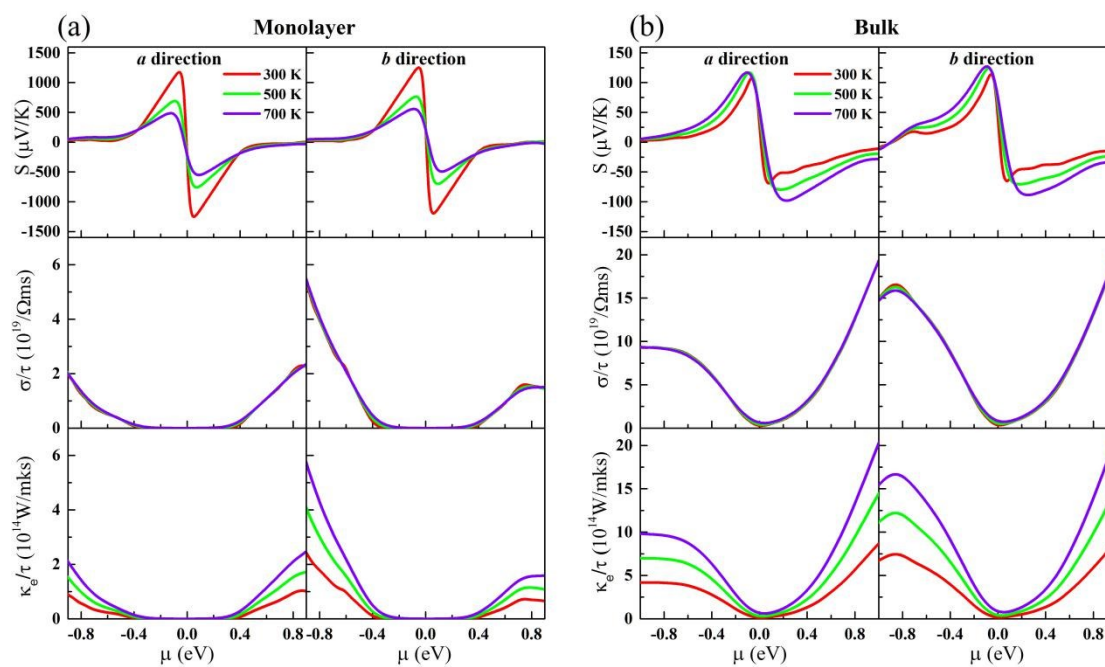
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## Electronic properties

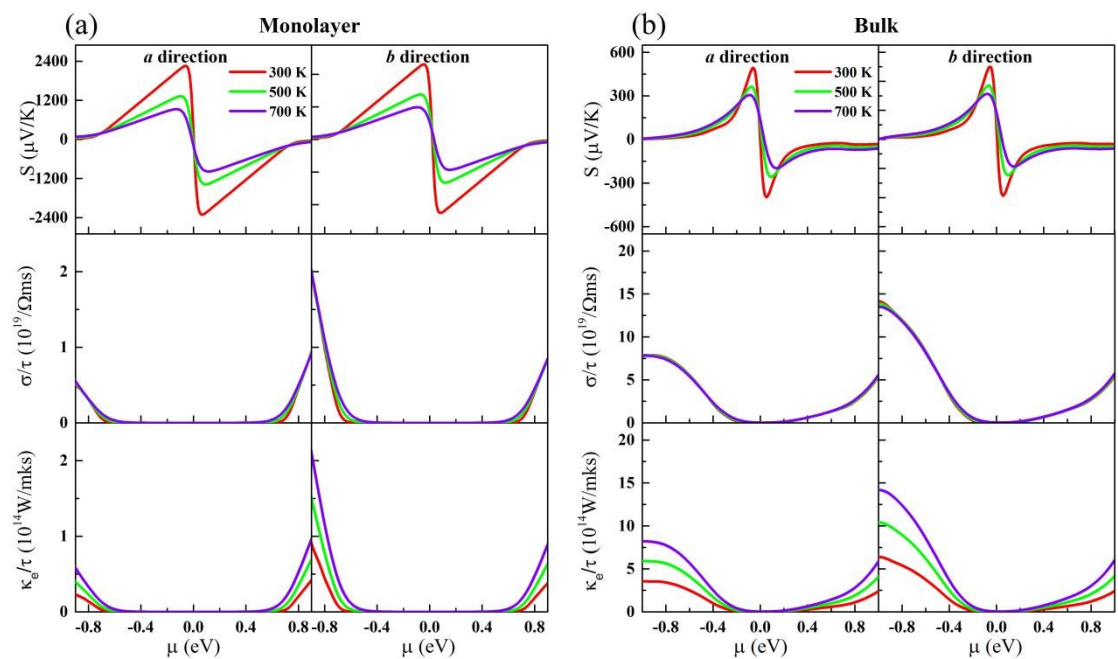


**Figure S1** Calculated band structures and DOSs for monolayer (left panel) and bulk (right panel)  $\text{CaP}_3$  with PBE and HSE06.

## The Electrical transport properties

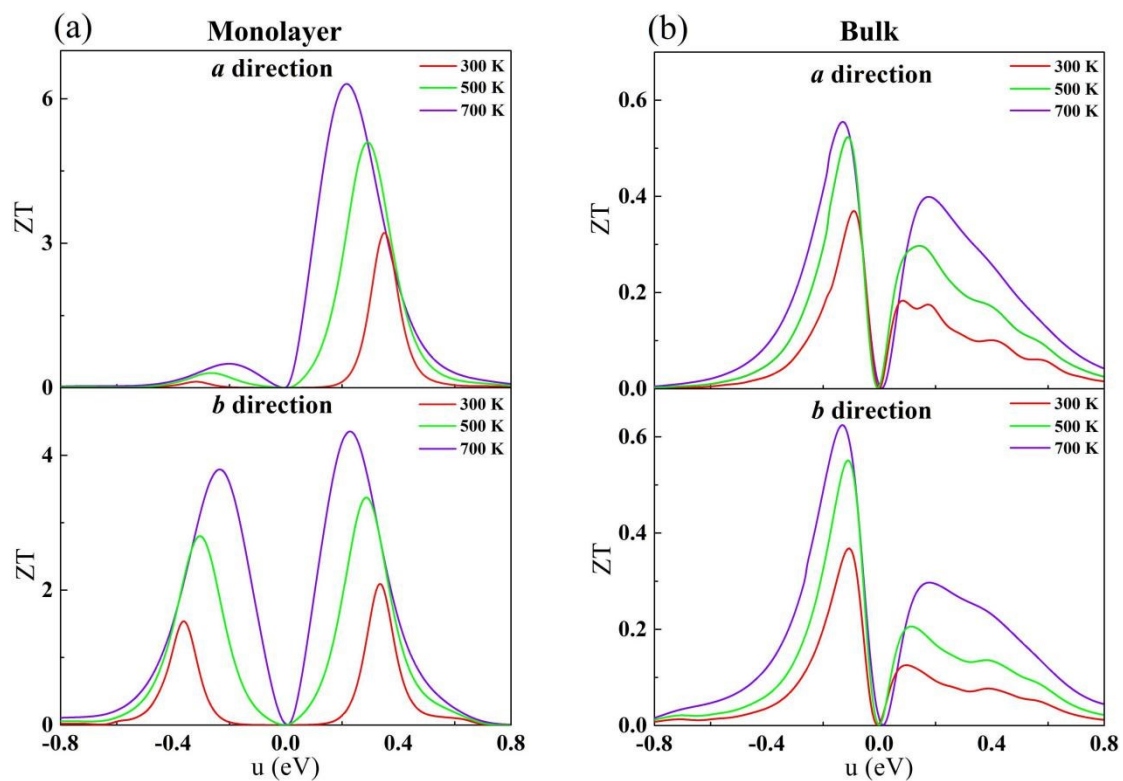


**Figure S2** Calculated electrical transport properties for monolayer and bulk  $\text{CaP}_3$  with PBE.

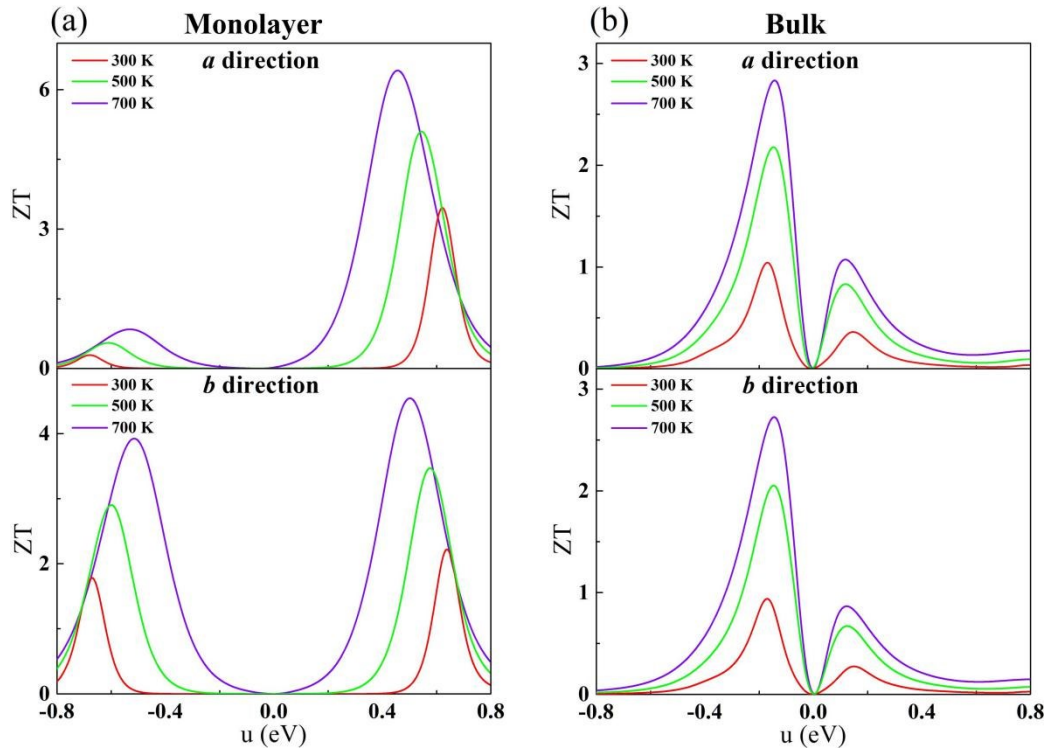


**Figure S3** Calculated electrical transport properties for monolayer and bulk  $\text{CaP}_3$  with PBE-Scissor.

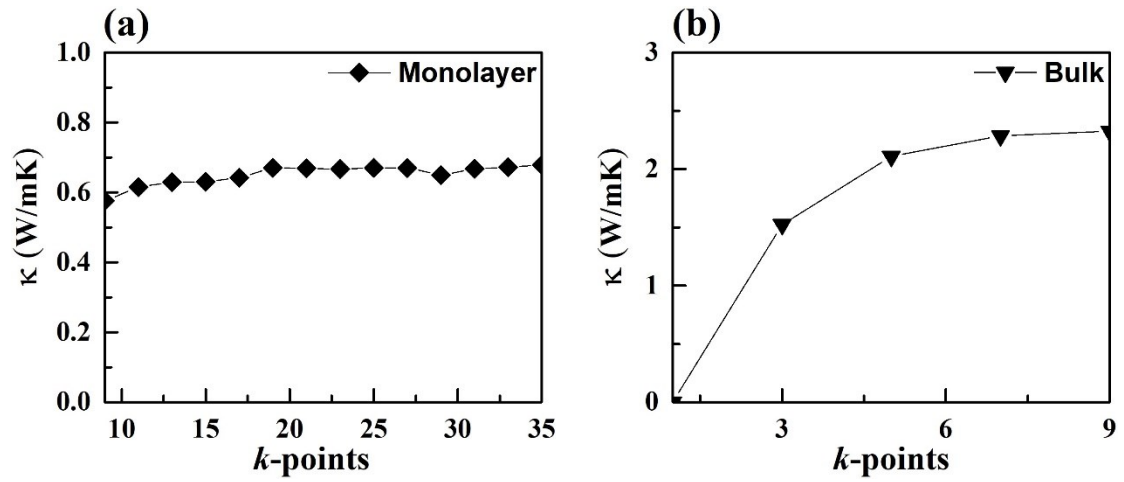
### The ZT values



**Figure S4** Calculated ZT values for monolayer and bulk  $\text{CaP}_3$  with PBE.



**Figure S5** Calculated ZT values for monolayer and bulk  $\text{CaP}_3$  with PBE-Sicssor.



**Figure S6** The lattice thermal conductivity along  $a$  direction as a function of  $k$ -points at 300 K for (a) monolayer and (b) bulk.

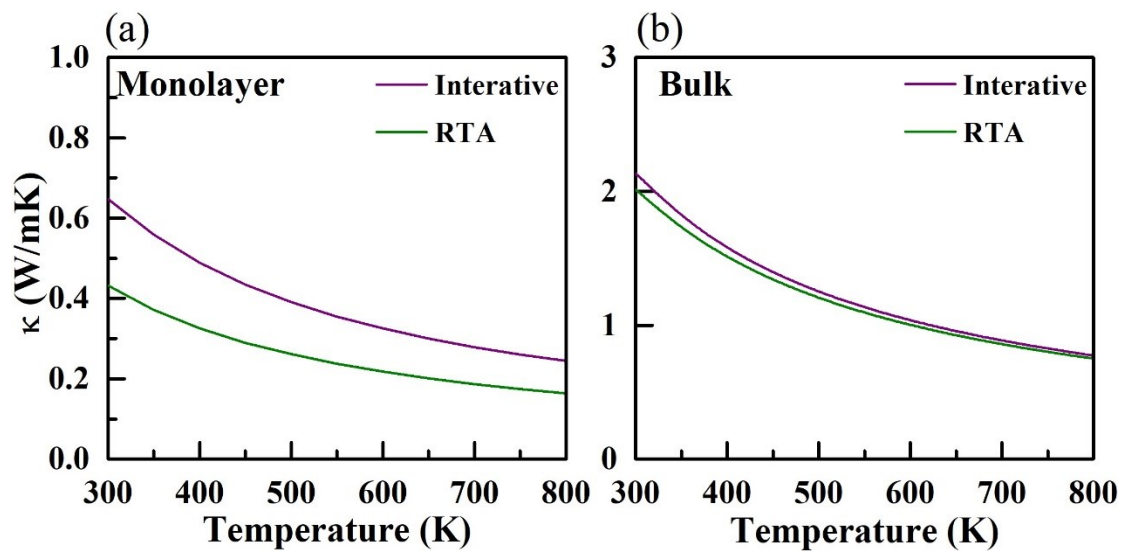


Figure S7 The lattice thermal conductivity of iterative and RTA for (a) monolayer and (b) bulk.