Electronic Supplementary Information (ESI)

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Title: Molecular dynamics study on thermal conductivity of KH2PO4 with vacancy defects

Table S1. Full Force-Field Parameters for the KDP (KH_2PO_4) Potential

The potential function used in this study is based on the model developed and validated by Yang et al. [Comput. Mater. Sci. 187 (2021) 110122]. The total potential energy is expressed as: $E_{pot} = E_{bond} + E_{angle} + E_{vdW} + E_{Coulomb} + E_{H\text{-}bond}$

(a) Atomic Partial Charges

Atom Type	Charge q_i (e)
K	+0.835
P	+0.461
O_1	-0.454
O_2	-0.506
H	+0.312

Note: O_1 and O_2 represent oxygen atoms within the hydroxyl group (P–OH) and the phosphoryl group (P=O) of the $[PO4]^{3-}$ tetrahedra, respectively, as defined in the potential model by Yang et al. [1].

(b) Covalent Bond and Angle Parameters (Harmonic)

Form: $E_{bond} = K_r(r - r_0)^2$; $E_{angle} = K_\theta(\theta - \theta_0)^2$

Interaction	r_0 (Å) / θ_0 (°)	K [kcal/(mol·Å²) or kcal/(mol·rad²)]

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Bond：P–O	1.600	430
Bond：O–H	1.037	500
Angle：O–P–O	109.5	25.0
Angle：P–O–H	110.5	148.8

(c) Hydrogen Bond Parameters (Specific H-bond part)[2]

Form: $E_{hyd} = \epsilon[5(\sigma/r)^{12} - 6(\sigma/r)^{10}]\cos^4 \theta$

Parameter	Value
Equilibrium well depth ϵ	17.5 kcal/mol
Zero-crossing distance σ	2.5 Å

(d) 9-6 Lennard-Jones Parameters (Van der Waals)

Form: $E_{vdW} = \epsilon_{ij}[2(\sigma_{ij}/r_{ij})^9 - 3(\sigma_{ij}/r_{ij})^6]$

Interaction (i - j)	$r_{0,ij}$ (Å)	$\epsilon_{0,ij}$ (kcal/mol)
$O_1 - O_1$	3.500	0.0385
$O_1 - O_2$	3.665	0.0451
$O_1 - K$	3.544	0.0882

Interaction (i - j)	$r_{0,ij}$ (Å)	$\epsilon_{0,ij}$ (kcal/mol)
$O_2 - O_2$	3.800	0.0560
$O_2 - K$	3.700	0.1050
$H - H$	1.098	0.0091
$H - P$	4.009	0.0012
$H - K$	3.194	0.0025
$P - P$	4.500	0.1750
$P - K$	4.164	0.1518
$K - K$	3.585	0.2030

References

[1] S. Yang, L. Zhang, H. Xie and W. Liu, Interaction potential function for the deformation analysis of potassium dihydrogen phosphate using molecular dynamics simulation, *Comput. Mater. Sci.*, 2021, 187, 110122.

[2] S. L. Mayo, B. D. Olafson and W. A. Goddard III, DREIDING: a generic force field for molecular simulations, *J. Phys. Chem.*, 1990, 94, 8897–8909.