Supplementary Information (SI) for Journal of Materials Chemistry C.

Supplementary Information for: First principles prediction unveils high-T_c superconductivity in YSc_2H_{24} cage structures under pressure

Truong-Tho Pham,[1,2] Viet-Ha Chu,[3] and Duc-Long Nguyen[4,2,*]

[1] *Laboratory of Magnetism and Magnetic Materials, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam*

[2] *Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam*

[3] *Department of Physics, TNU-University of Education, Thai Nguyen, Vietnam*

[4] *Simulation in Materials Science Research Group, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Viet Nam*

* nguyenduclong@vlu.edu.vn

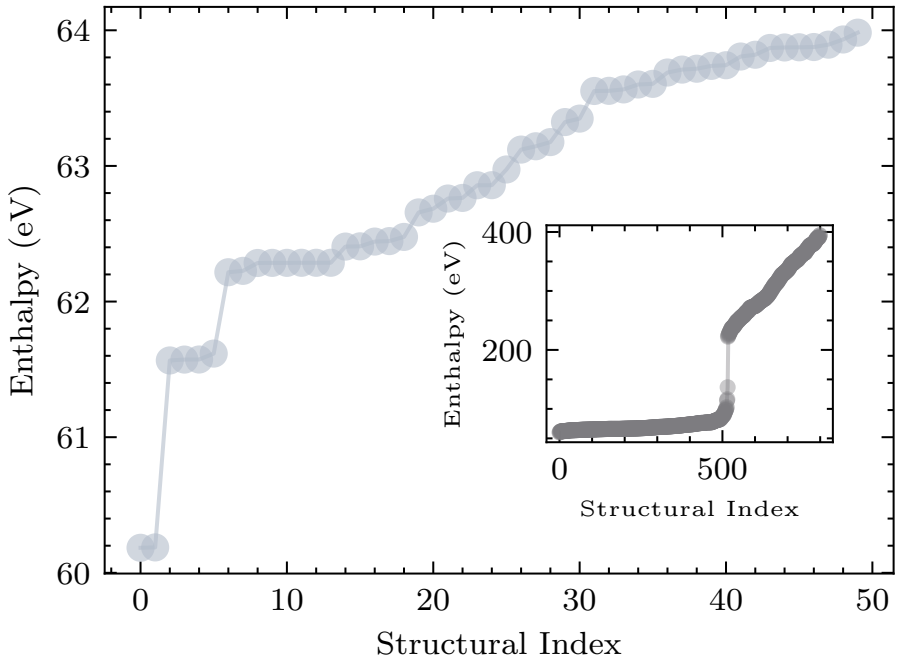

Fig. S 1. (Color online) The enthalpy of the 50 crystal structures with the lowest value. Plateaus indicate discovered structures with the same space group. At 300 GPa, the $P6/mmm$ structure has the lowest enthalpy. The inset figure depicts a more comprehensive view of the enthalpy range of up to 800 lowest enthalpy structures.

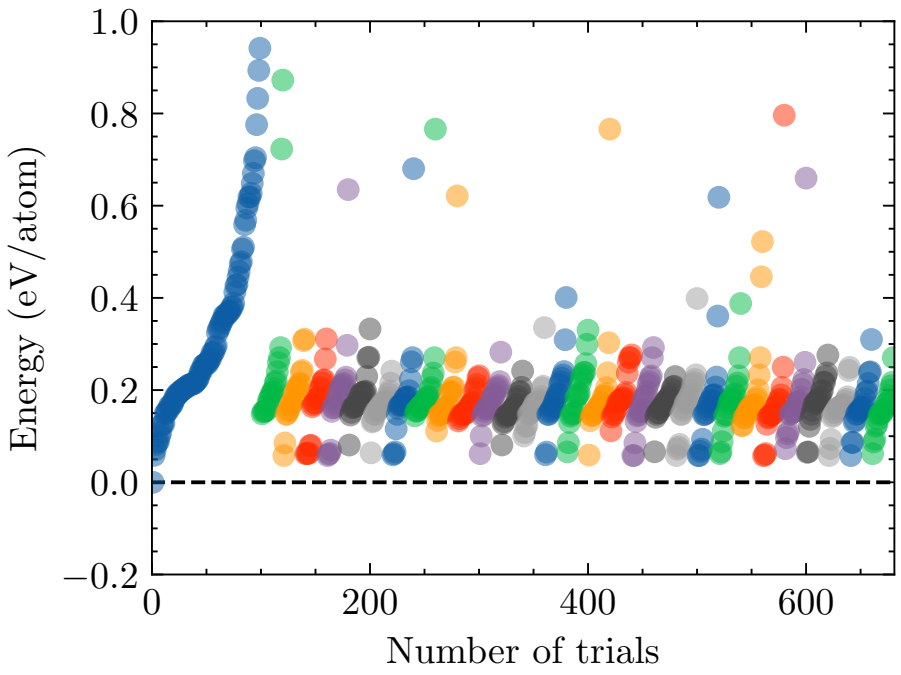

Fig. S 2. (Color online) Evolutionary algorithm crystal structure prediction for YSc_2H_{24}. From left to right, different crystal generations are depicted in different colors. The first generation employed larger random structures to increase the success rate of crystal structure searching. We plot only structures that have energy within 1 eV/atom of the lowest energy structure.

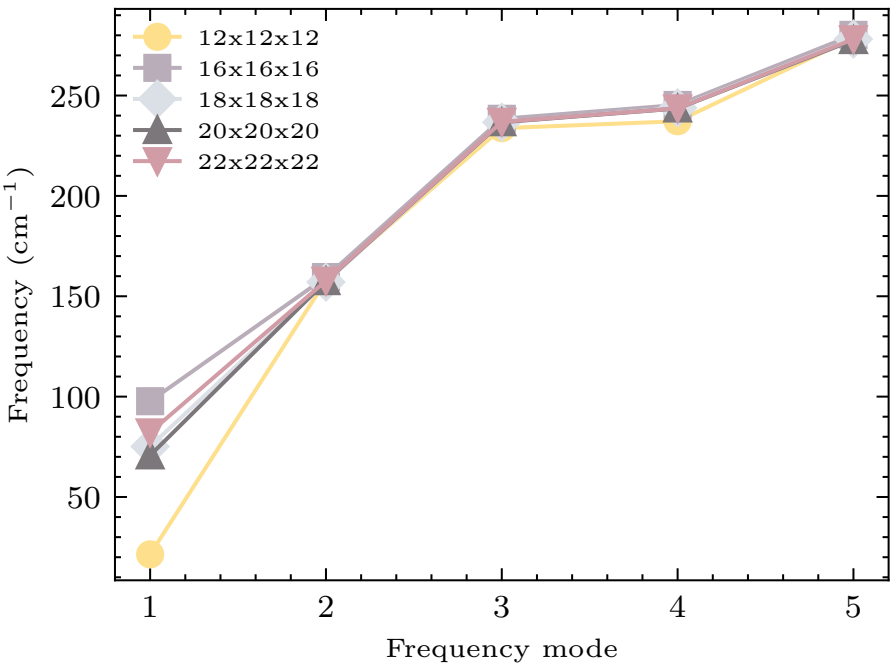

Fig. S 3. (Color online) Phonon frequencies of the first 5 phonon branches calculated at 310 GPa. Convergence to within a few cm^{-1} required a dense k-point mesh of 18×18×18. Higher frequency modes are easier to converge, while the first mode is quite sensitive to k-point sampling.

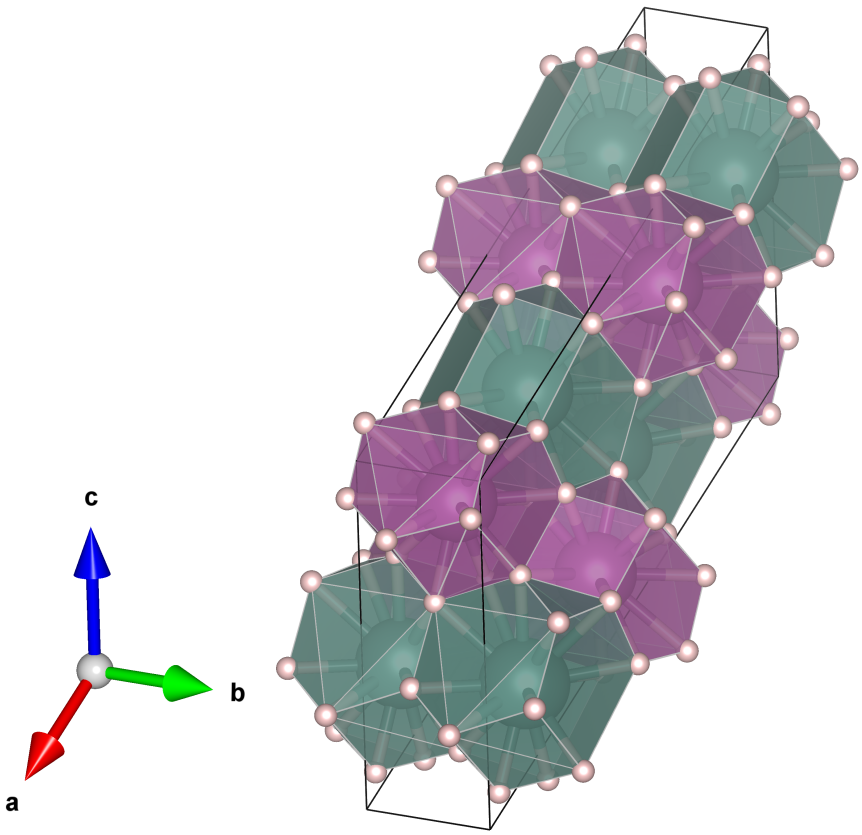

Fig. S 4. Crystal structure of $C2/m$ $Y_2Sc_2H_{12}$ at 310 GPa

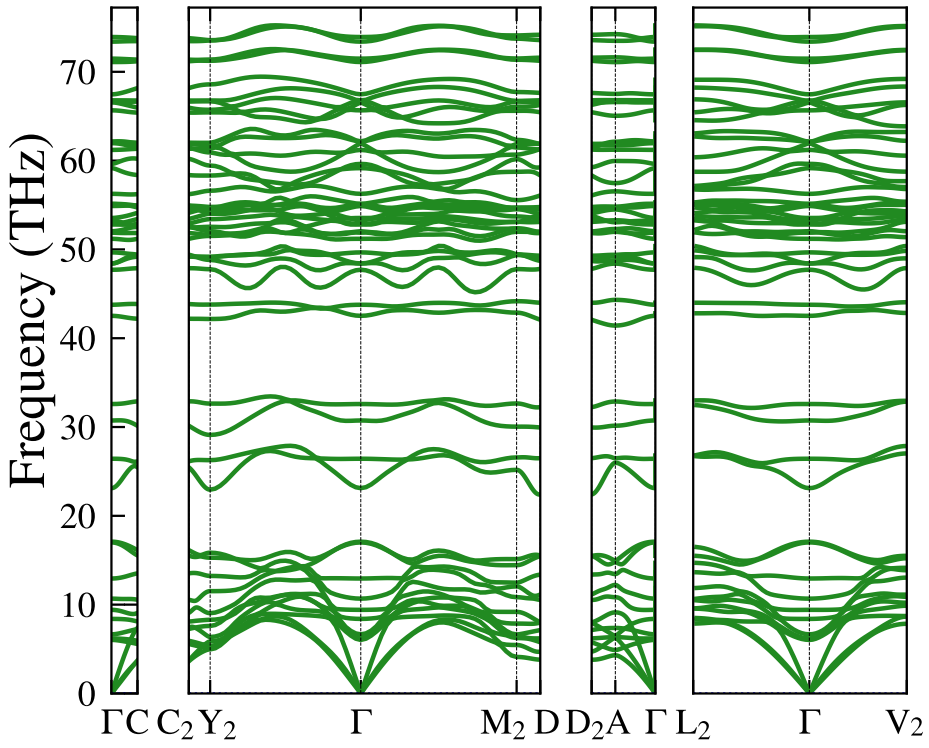

Fig. S 5. Phonon dispersion of $C2/m$ $Y_2Sc_2H_{12}$ at 310 GPa

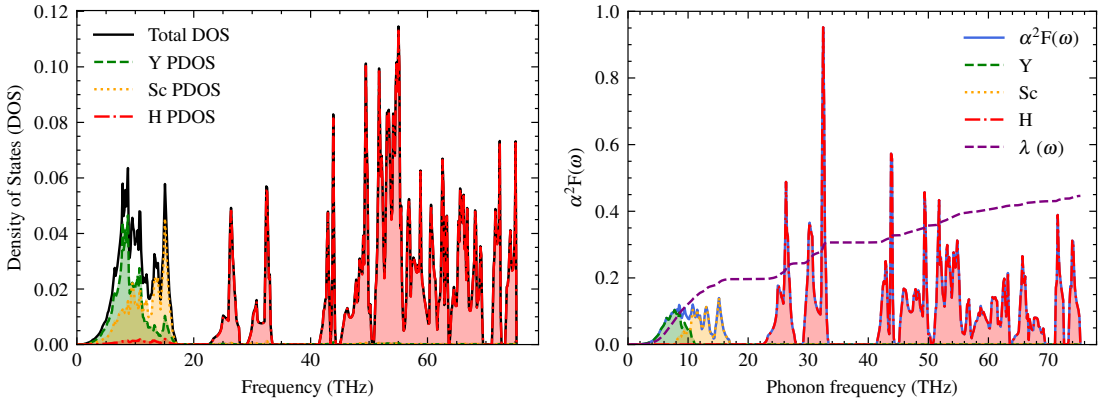

Fig. S 6. Phonon DOS and the Eliashberg phonon spectral function $C2/m$ $Y_2Sc_2H_{12}$ at 310 GPa

SP#	SPname	a	b	c	α	β	γ
27	P6/mmm	4.600610	4.600610	3.242590	90.0	90.0	120.0
Atom	Element	Multiplicity	Wyckoff	x	y	z	Occupancy
Y1	Y	1	b	0.00000	0.00000	0.50000	1.00000
Sc1	Sc	2	c	0.33333	0.66667	0.00000	1.00000
H1	H	6	m	0.76309	0.52618	0.50000	1.00000
H2	H	6	j	0.22871	0.00000	0.00000	1.00000
H3	H	12	n	0.37987	0.00000	0.29054	1.00000

TABLE I. Calculated crystal structure of YSc_2H_{24} at 310 GPa. Lattice parameters are given in units of Å

SP#	SPname	a	b	c	α	β	γ
12	C2/m	9.649840	2.459980	5.706100	90.0	125.913470	90.0
Atom	Element	Multiplicity	Wyckoff	x	y	z	Occupancy
Y1	Y	4	i	0.12851	0.00000	0.74730	1.00000
Sc1	Sc	4	i	0.37547	0.00000	0.75185	1.00000
H1	H	4	i	0.80352	0.00000	0.88906	1.00000
H2	H	4	i	0.54397	0.00000	0.43313	1.00000
H3	H	4	i	0.87433	0.00000	0.56599	1.00000
H4	H	4	i	-0.03301	0.00000	0.06515	1.00000
H5	H	4	i	0.71780	0.00000	0.59874	1.00000
H6	H	4	i	0.38903	0.00000	0.05342	1.00000

TABLE II. Calculated crystal structure of $Y_2Sc_2H_{12}$ at 310 GPa. Lattice parameters are given in units of Å