Supplementary information for Prediction of radon-silica systems in the Earth's mantle

Kai Hu[1], Yixing Geng[3], Yanying Zhao[3], Yuqiu Gu[4,*], Jinqing Yu[2,*], and Xueqing Yan[3,5,6,*]

1 School of Mathematics and Physics, Nanjing Institute of technology, Nanjing 211167, China

2 Hunan Provincial Key Laboratory of High-Energy Scale Physics and Applications, School of Physics and Electronics, Hunan University, Changsha 410082, China

3 State Key Laboratory of Nuclear Physics and Technology, and Key Laboratory of HEDP of the Ministry of Education, CAPT, Peking University, Beijing 100871, China

4 Shanghai Institute of Laser Plasma, Shanghai 201800, China

5 Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China

6 Guangdong Laser Plasma Institute, Guangzhou 510540, China

E-mail: *yqgu@caep.cn; *jinqing.yu@hnu.edu.cn; *x.yan@pku.edu.cn

We tested the standard PBE functional and PBE with DFT-D3 dispersion correction, as shown in Figure S1. We calculated the electronic density of states for the *Fd*-3*m* and $P4_1$ structures, as shown in Figure S2. The Rn-*p*

electrons mainly contribute to states around the Fermi level. The PBE functional underestimates the band gaps of semiconductors and insulators. Therefore, we used a hybrid functional with dispersion corrections to calculate the electronic band structure, resulting in a more accurate band gap, as shown in Figure S3. Detailed elastic constants and stiffness tensor Cij are presented in Table S1 and S2.

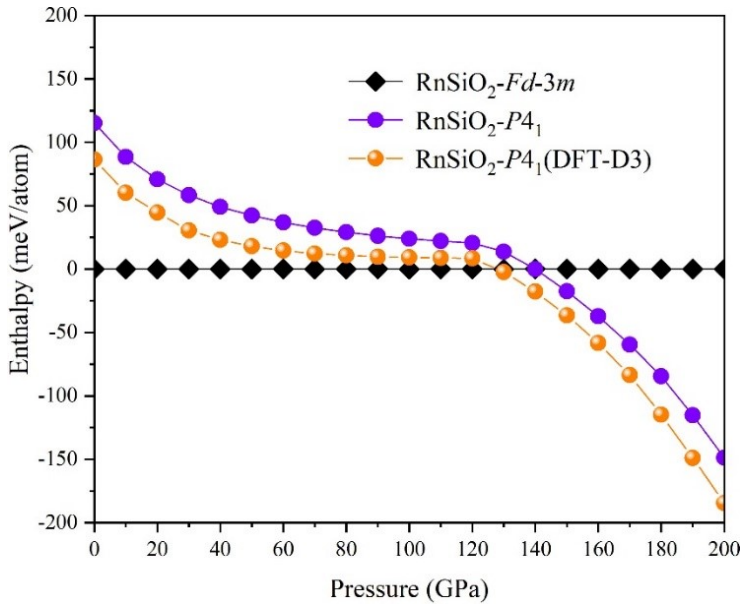

Figure S1. The dispersion corrected relative enthalpy of the *Fd*-3*m* and $P4_1$ phases.

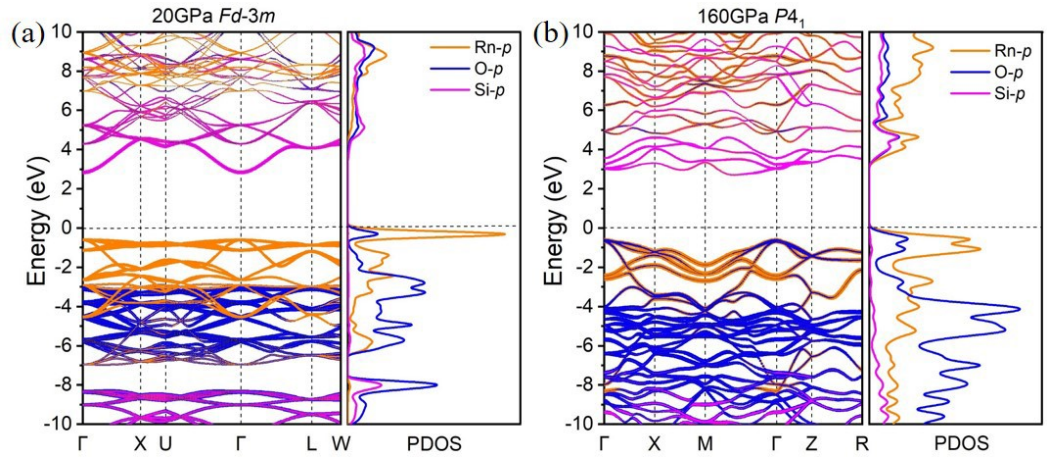

Figure S2. Electronic band structure and corresponding PDOS for (**a**) the *Fd*-3*m* phase at 20 GPa, and (**b**) the $P4_1$ phase at 160 GPa. The Rn-*p*, O-*p*, and Si-*p* electrons are drawn in orange, blue, and pink, respectively.

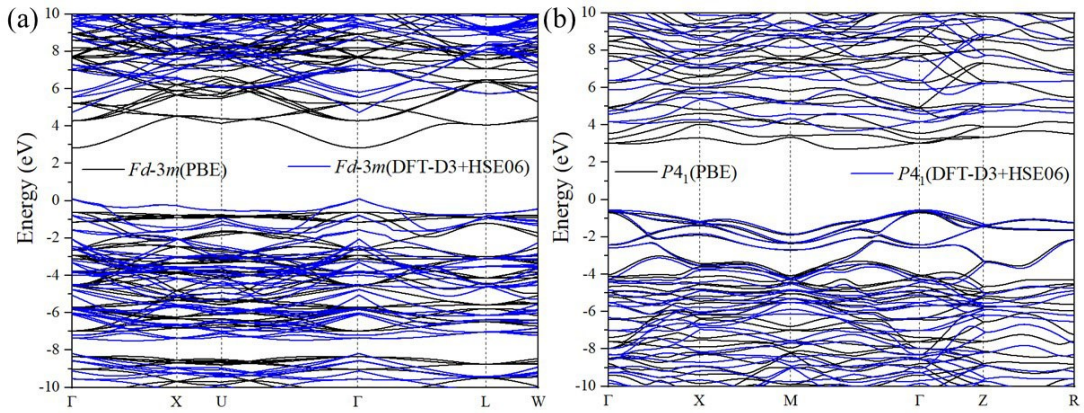

Figure S3. Calculated phonon band structures of (a) the *Fd*-3*m* phase with PBE and DFT-D3+HSE06 at 20 GPa, and (b) the $P4_1$ phase with PBE and DFT-D3+HSE06 at 160 GPa.

Table S1. Three independent elastic constants and stiffness tensor C_{ij} of the *Fd*-3*m* phase.

Elastic Constants:

C11	C12	C12	0	0	0
C12	C11	C12	0	0	0
C12	C12	C11	0	0	0
0	0	0	C44	0	0
0	0	0	0	C44	0
0	0	0	0	0	C44

Stiffness Tensor C_ij (in GPa):

305.530	142.815	142.815	0.000	0.000	0.000
142.815	305.530	142.815	0.000	0.000	0.000
142.815	142.815	305.530	0.000	0.000	0.000
0.000	0.000	0.000	104.363	0.000	0.000
0.000	0.000	0.000	0.000	104.363	0.000
0.000	0.000	0.000	0.000	0.000	104.363

Table S2. Seven independent elastic constants and stiffness tensor C_{ij} of the $P4_1$ phase.

Elastic Constants:

C11	C12	C13	0	0	C16
C12	C11	C13	0	0	-C16
C13	C13	C33	0	0	0
0	0	0	C44	0	0
0	0	0	0	C44	0
C16	-C16	0	0	0	C66

Stiffness Tensor C_ij (in GPa):

540.643	186.429	338.811	0.000	0.000	-19.991
186.429	540.643	338.811	0.000	0.000	19.991
338.811	338.811	552.326	0.000	0.000	-0.000
0.000	0.000	0.000	226.154	0.000	0.000
0.000	0.000	0.000	0.000	226.154	0.000
-19.991	19.991	-0.000	0.000	0.000	128.937