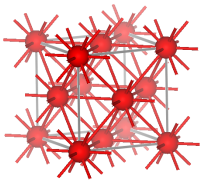
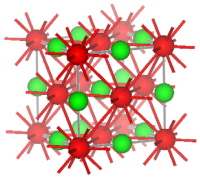
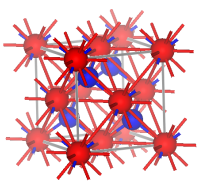
Supplemental Material

for the paper "Solubility of deuterium and hydrogen in fcc iron at high pressures and temperatures" by V. E. Antonov, V. M. Gurev, V. I. Kulakov, M. A. Kuzovnikov, I. A. Sholin, and V. Y. Zuykova

TABLE SI. Compositions and crystal structures used in calculations of the present paper. The relaxed lattice parameters and enthalpies refer to $T = 0$ K and $P = 0$ GPa. In the crystal structures schematically shown in the leftmost column, the metal atoms are red, H(octa) atoms are green, and H(tetra) atoms are blue. The accuracy in calculating the lattice parameters and enthalpies is about 1%. The results in the table are not rounded so that they can be used to calculate ΔV and ΔH for different phases of the same metal, which can be done with higher accuracy due to the mutual compensation of systematic calculation errors.

Structure & space group	Atomic positions (unrelaxed)		Fe-H	Ni-H	Pd-H	Rh-H
fcc-Me $Fm\bar{3}m$ 	Me 0 0 0	Lattice parameters (Å)	a=3.440	a=3.533	a=3.934	a=3.894
		Volume V (Å^3/atom Me)	10.17	11.03	15.22	14.77
		Enthalpy H (eV/atom Me)	-865.200	-1354.372	-798.653	-606.861
fcc-MeH(octa) $Fm\bar{3}m$ 	H(octa) 1/2 1/2 1/2 Me 0 0 0	Lattice parameters (Å)	a=3.638	a=3.745	a=4.105	a=4.077
		Volume V (Å^3/atom Me)	12.04	13.13	17.30	16.94
		Enthalpy H (eV/atom Me)	-881.107	-1370.321	-814.731	-622.743
		$\langle\hbar\omega\rangle^{\mathrm{H}}_{\mathrm{octa}}$ (meV)	114	79	51	65
fcc-MeH(tetra) $F\bar{4}3m$ 	H(tetra) 1/4 1/4 1/4 Me 0 0 0	Lattice parameters (Å)	a=3.755	a=3.858	a=4.218	a=4.189
		Volume V (Å^3/atom Me)	13.24	14.36	18.76	18.38
		Enthalpy H (eV/atom Me)	-880.765	-1370.300	-814.768	-622.656
		$\langle\hbar\omega\rangle^{\mathrm{H}}_{\mathrm{tetra}}$ (meV)	183	147	124	137

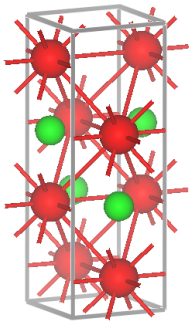
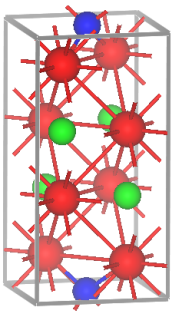
Me_2H(octa) $P4/nmm$ 	H(octa) 1/2 0 3/8 Me 1/2 0 5/8 Me 0 1/2 7/8	Lattice parameters (Å)	a=2.515 c=7.042	a=2.589 c=7.241	a=2.828 c=8.180	a=2.814 c=8.030
		Volume V (Å^3/atom Me)	11.13	12.13	16.36	15.90
		Enthalpy H (eV/atom Me)	-873.141	-1362.339	-806.722	-614.791
$Me_8H(octa)_4H(tetra)$ $P\bar{4}2m$ 	H(tetra) 1/2 1/2 0 H(octa) 1/4 1/4 5/8 Me 1/4 3/4 1/8 Me 1/4 1/4 3/8	Lattice parameters (Å)	a=3.589 c=7.145	a=3.699 c=7.321	a=4.047 c=8.197	a=4.030 c=8.051
		Volume V (Å^3/atom Me)	11.50	12.52	16.78	16.34
		Enthalpy H (eV/atom Me)	-875.080	-1364.313	-808.733	-616.733

TABLE SII. Calculated hydrogen-induced volume expansions of metal lattice β_H^O and β_H^T for hydrogen at the O and T interstitial sites, respectively, of the fcc metal lattice. $\beta_H^O = V$(fcc-MeH(octa)) – V(fcc-Me) and $\beta_H^T = 8\{V(P\bar{4}2m\text{-}Me_8H(octa)_4H(tetra)) - V(P4/nmm\text{-}Me_2H(octa))\}$, where V are the atomic volumes from Table SI.

System	β_H^O, Å^3/atom H		β_H^T, Å^3/atom H
	DFT calculation	Experiment	DFT calculation
Fe-H	1.86	2.21 @ 988 K [27]	2.94
Ni-H	2.10	2.20 @ 120 K [1,20]	3.15
Pd-H	2.07	2.47 @ 77 K [1]	3.35
Rh-H	2.18	2.40 @ 120 K [1,20]	3.59

FIG. S1. Calculated phonon dispersions and densities of states for the fcc-MeH(octa) and fcc-MeH(tetra) crystal structures.