Supplementary Materials: Study of anharmonicity in Zirconium Hydrides using inelastic neutron scattering and ab-initio computer modeling

Jiayong Zhang [1,2], Yongqiang Cheng [2], Alexander I. Kolesnikov [2], Jerry Bernholc [1,3], Wenchang Lu [1,3], Anibal J. Ramirez-Cuesta [2,*]

1. Eigen states based on 2D Schrödinger equation

We have sampled 2D potential energy surfaces of all three materials and solved the according Schrödinger equations as shown in Eq. 2 in the original article. The eigenstates with the lowest 15 energies, which represent the wavefunctions of the single hydrogen/deuterium atom, are plotted in Fig. S1. The black texts above the green background are indicating eigenfrequencies in meV, and areas in blue/red are wavefunctions.

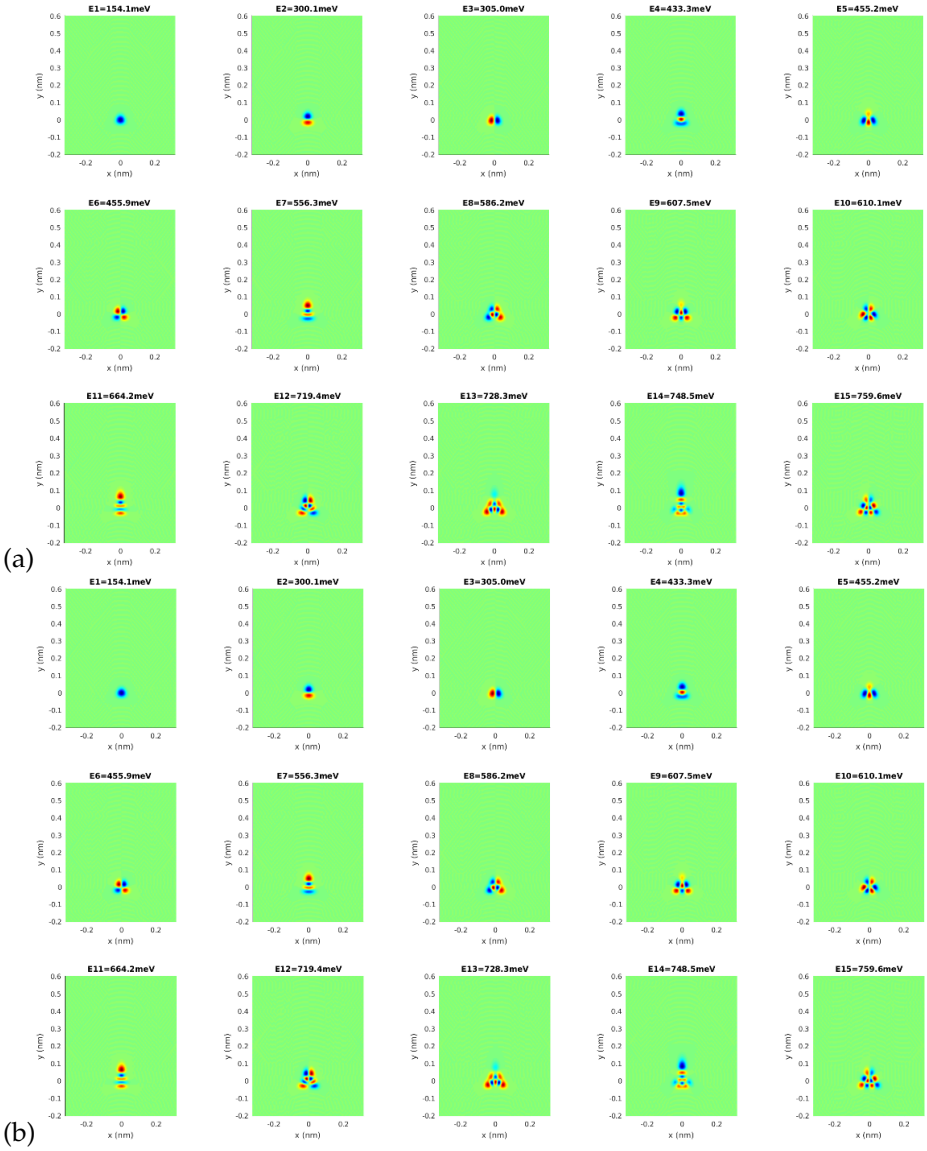
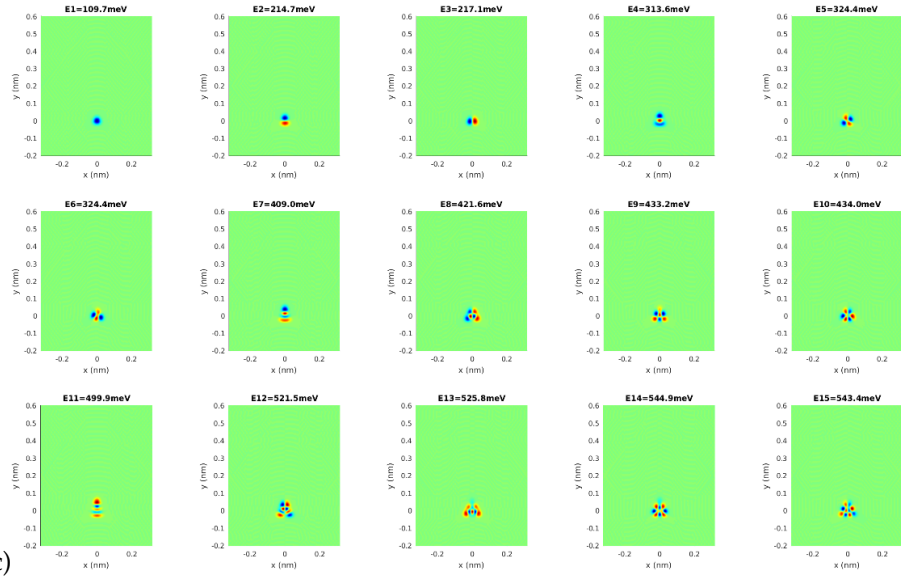


Figure S1. *Cont.*



(c)

Figure S1. First fifteen eigenfrequencies and wavefunctions of H(D) for: (a) (112) plane of ϵ-ZrH_2, (b) (-112) plane of ZrH, and (c) (-112) plane of ZrD.

2. Comparisons of eigenfrequencies between ZrH_x

Based on the eigenfrequencies in Fig. S1 (and more not plotted), we plot in Fig. S2 the differences of eigenfrequencies below 1000 meV for three materials.

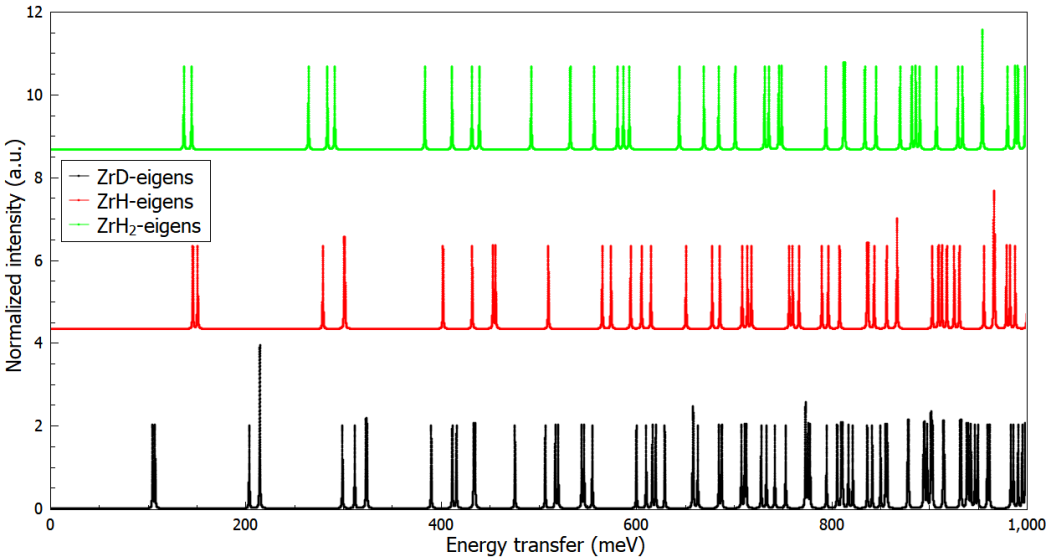


Figure S2. Comparisons of eigenfrequencies by solving Schrödinger equations for ZrH_x in the energy range below 1000 meV.

3. The probability distribution of H atoms in ZrH_2

According to quantum theory, the probability distribution of a particle is the modulus square of the particle's wavefunctions:

$$\rho(\mathbf{r}) = c|\psi(\mathbf{r})|^2 \tag{1}$$

where c is the normalization factor. To quantitatively obtain the spatial distribution of the hydrogen atom, the (unnormalized) probability distributions of hydrogen in (112) plane along x and y directions (with y=0 and x=0, respectively) in ZrH_2 are plotted in Fig. S3. The dashed lines are indicating the full width at half maximum.

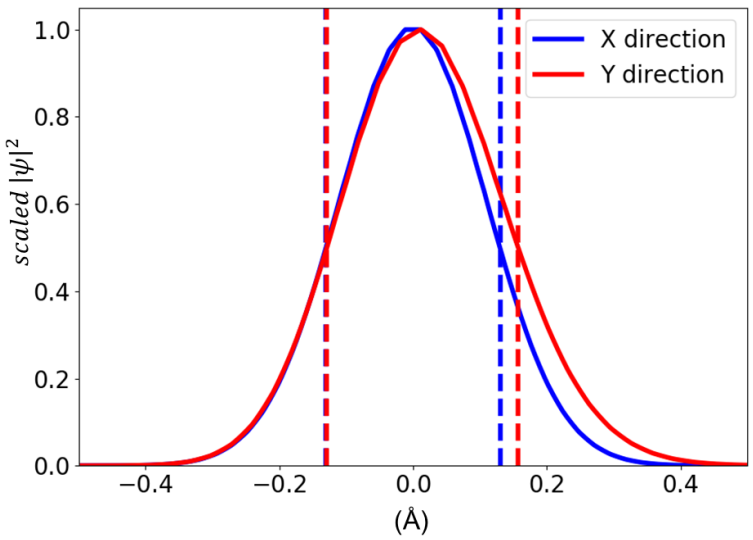


Figure S3. Unnomalized probability distributions of H atom in ZrH_2 in (112) plane along x (blue) and y (red) directions, where the dashed lines are indicating full width at half maximum (FWHM).