Supporting Information

First-principles theoretical studies and nano-calorimetry experiments on solid-state alloying of Zr-B

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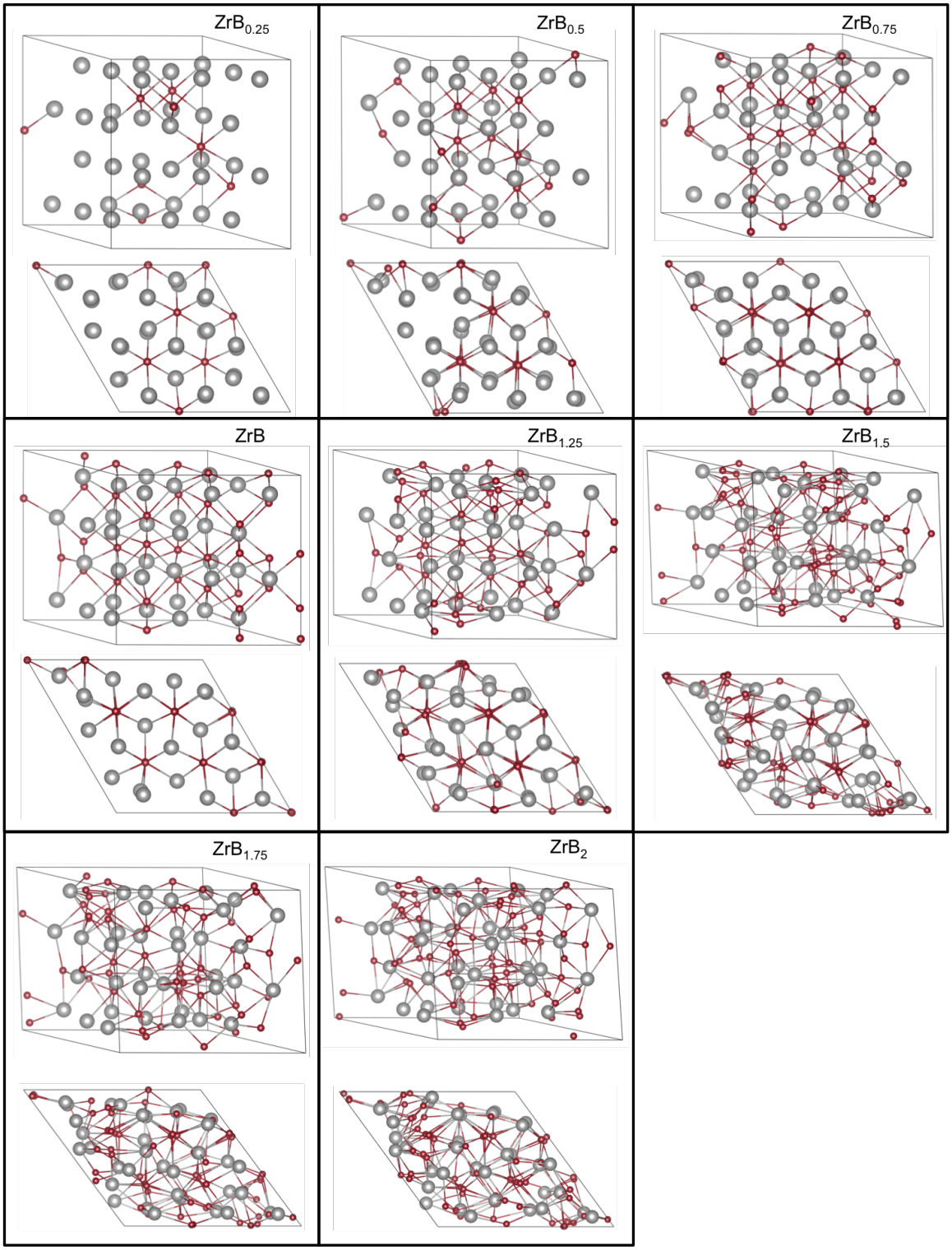

Figure S1. Structural evolution upon insertion of B in Zr lattice: prospect view (top) and plan view (bottom) at each concentration.

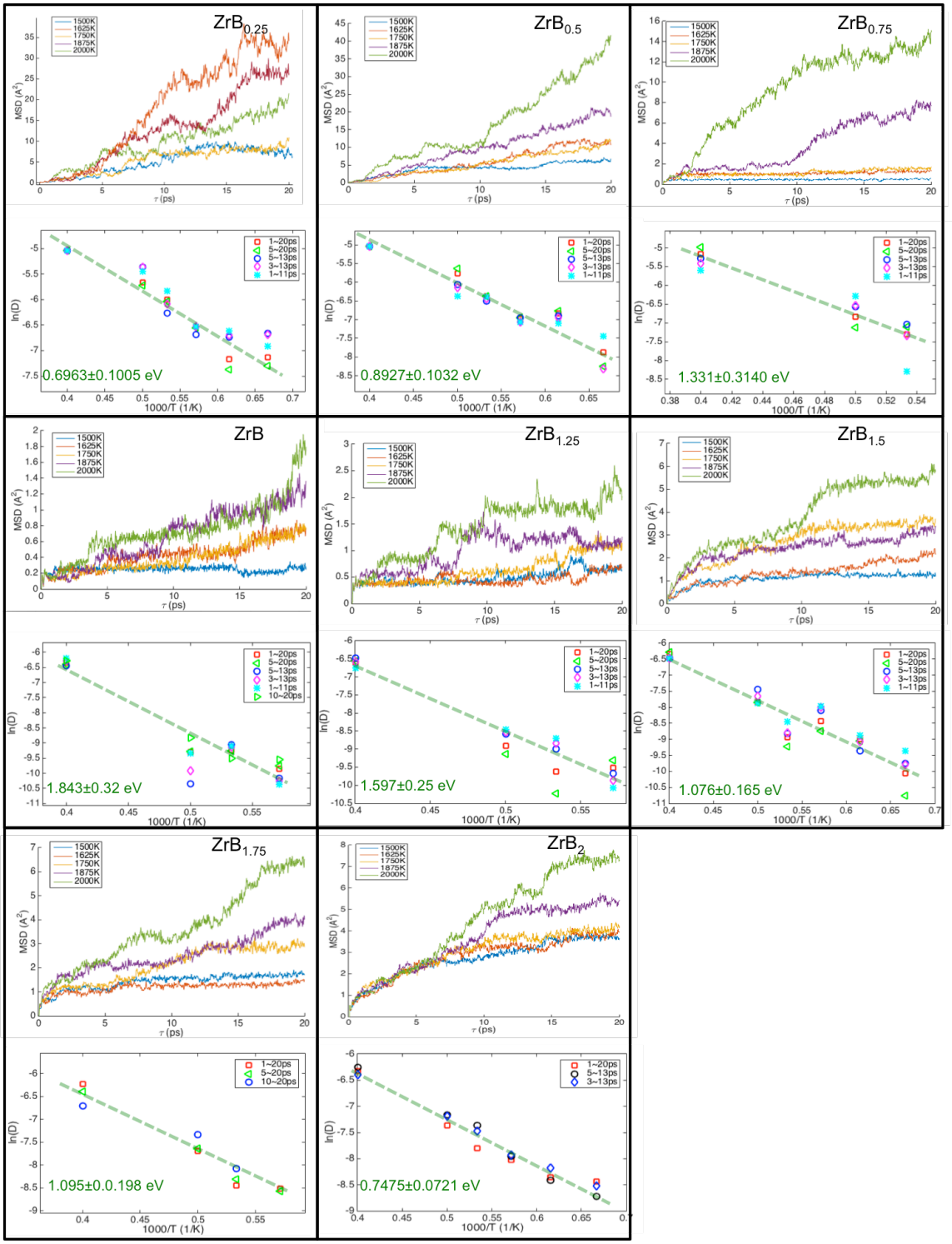

Figure S2. Mean square displacement (MSD) vs. simulation time (top) and diffusivity vs. reciprocal temperature (bottom) for various concentrations. The activation energy of B diffusion for each concentration has been obtained by considering the Arrhenius relation and indicated in the diffusivity plots. MSD plots are not perfectly linear so we use different sample times to obtain

diffusivity at each temperature. This calculation method and the non-linearity in the MSD plots create the error in the activation energy at each concentration.