

Description of Additional Supplementary Files

Supplementary Data 1. The AIMD configurations of PdRhMoFeMn HEMs under the first frame, and the last frame (i.e., 300, 400, and 500 K) for molecular dynamics simulations.

Supplementary Data 2. The atomic coordinates of the optimized computational models of PdRhMoFeMn HEMs under the first frame and the last frame for electronic structure calculations.