

Supporting information for:

The role of distinct metal cocatalysts in tuning β -ZrNBr for diverse photocatalytic applications

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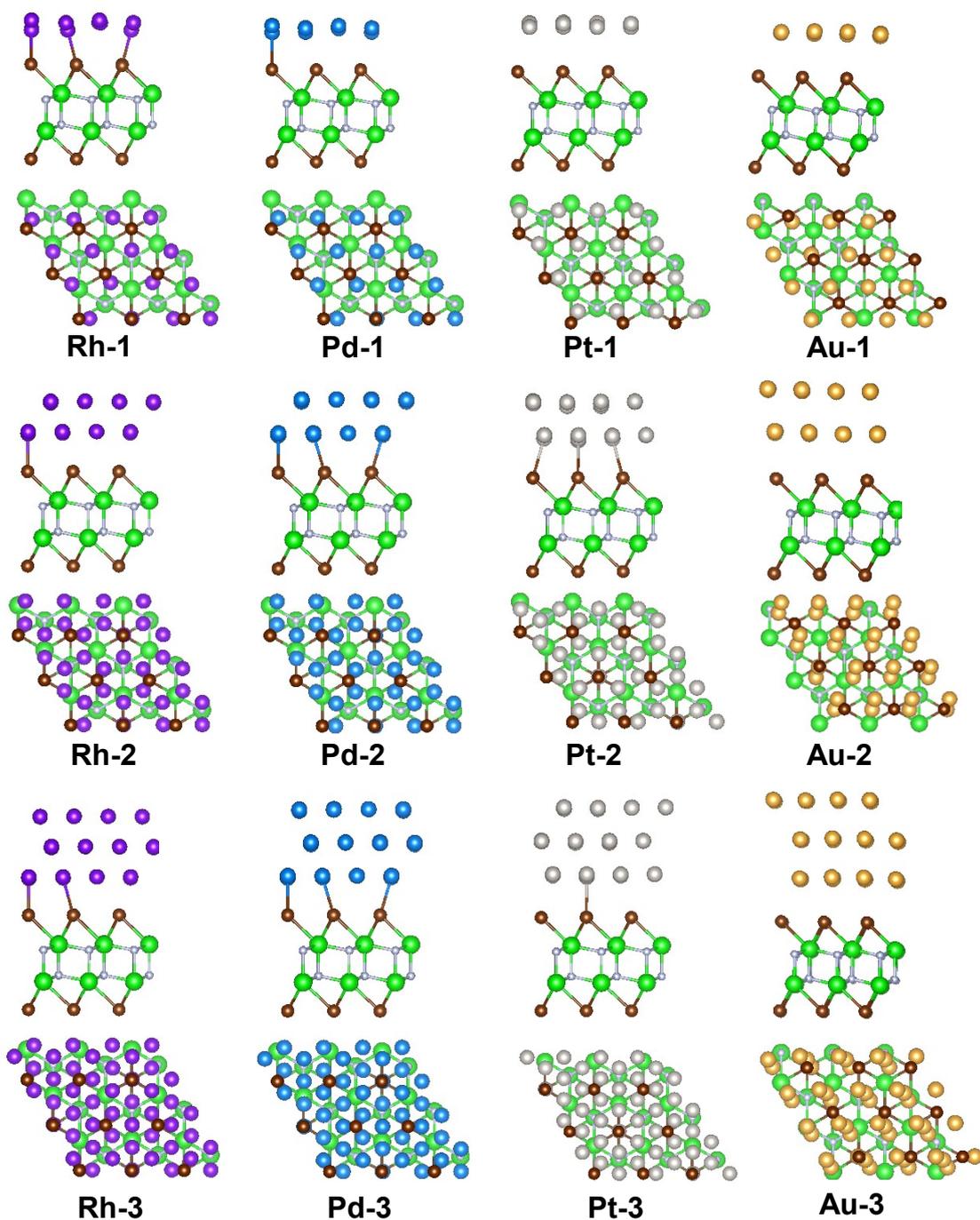


Fig. S1 Side and top views of the optimized structures for all the M/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), purple (Rh), blue (Pd), silver (Pt), and yellow (Au).

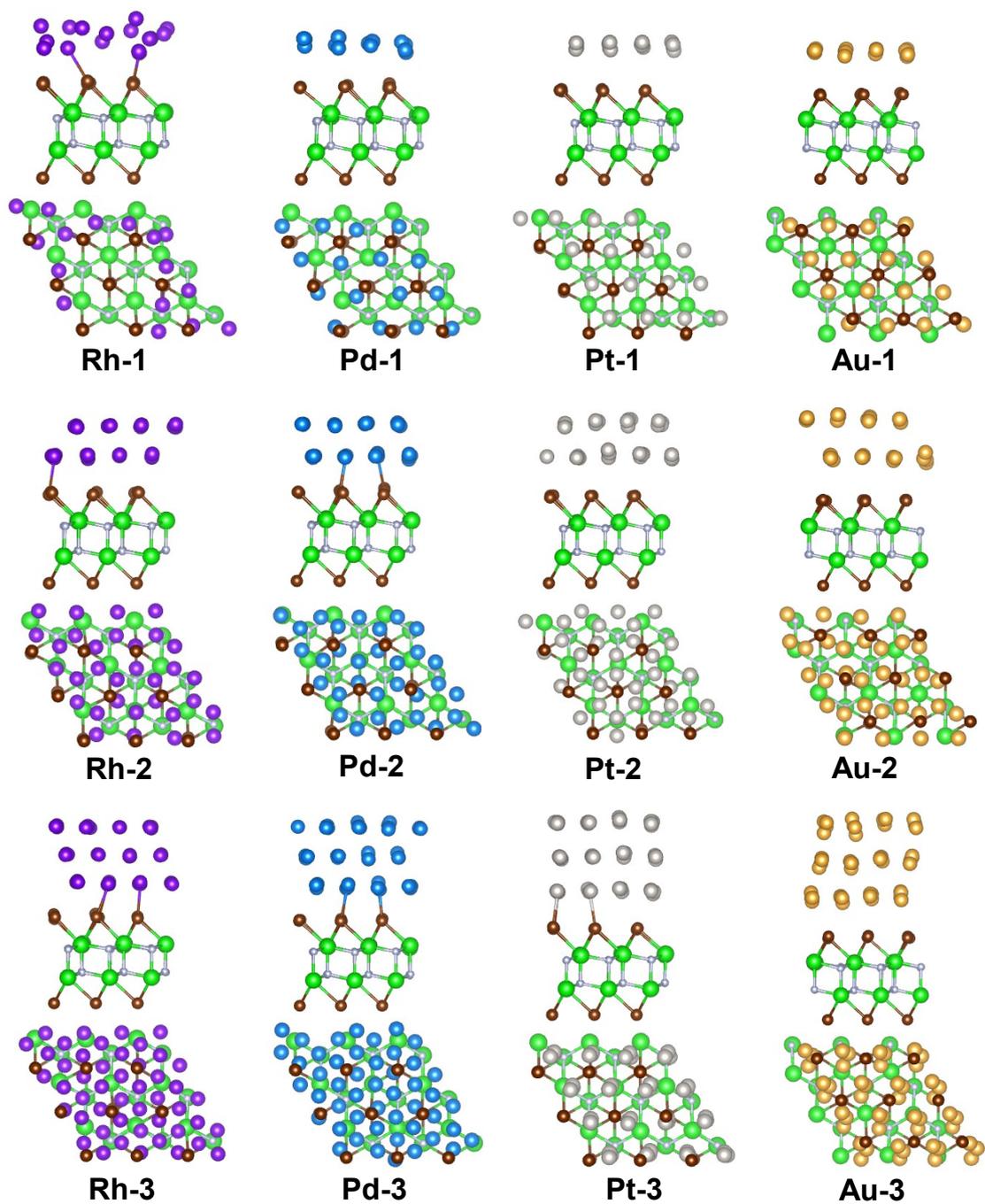


Fig. S2 Final AIMD snapshots (side and top views) of the studied M/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), purple (Rh), blue (Pd), silver (Pt), and yellow (Au).

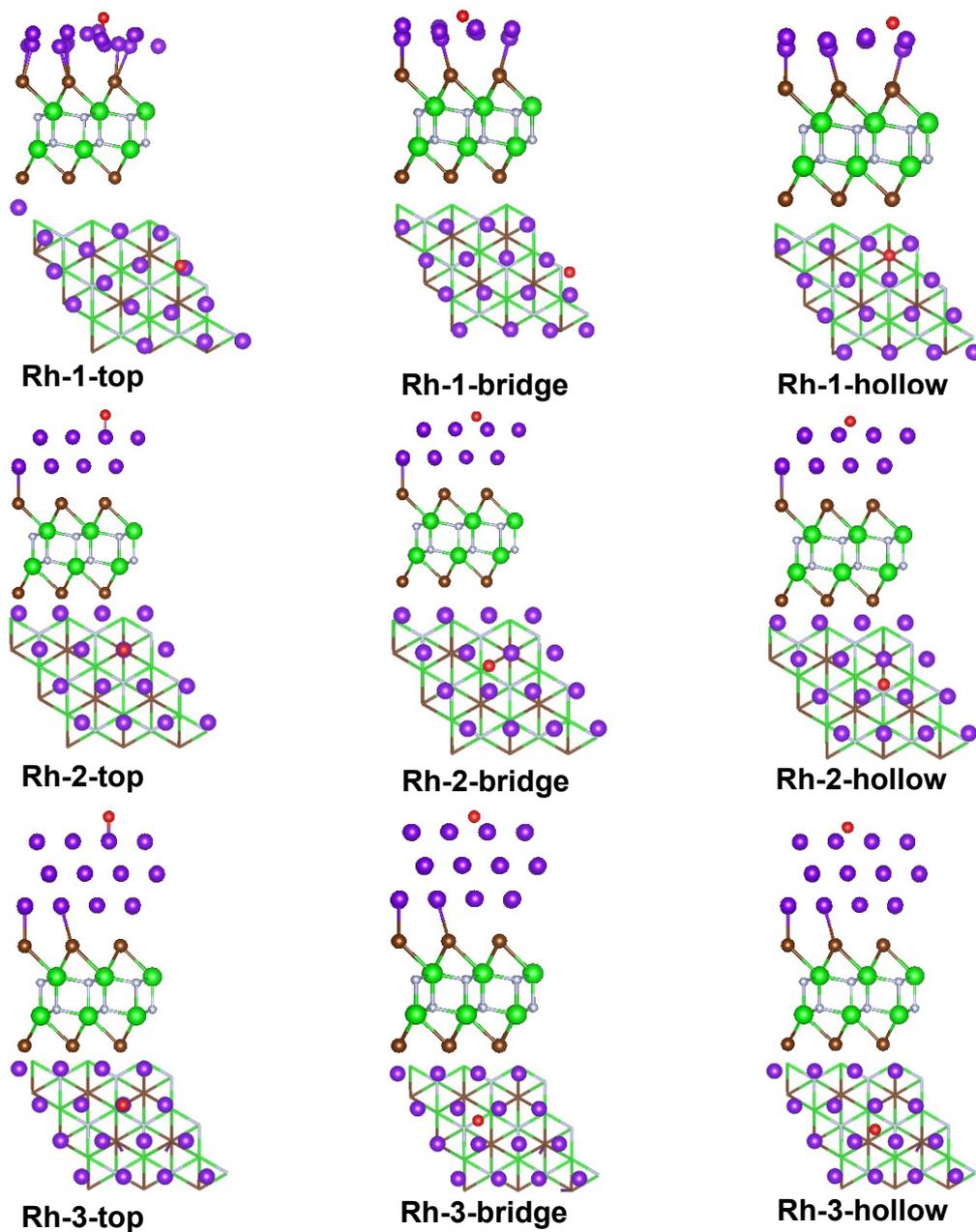


Fig. S3 Side and top views of the optimized structures for H adsorbed Rh/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), purple (Rh), and red (H).

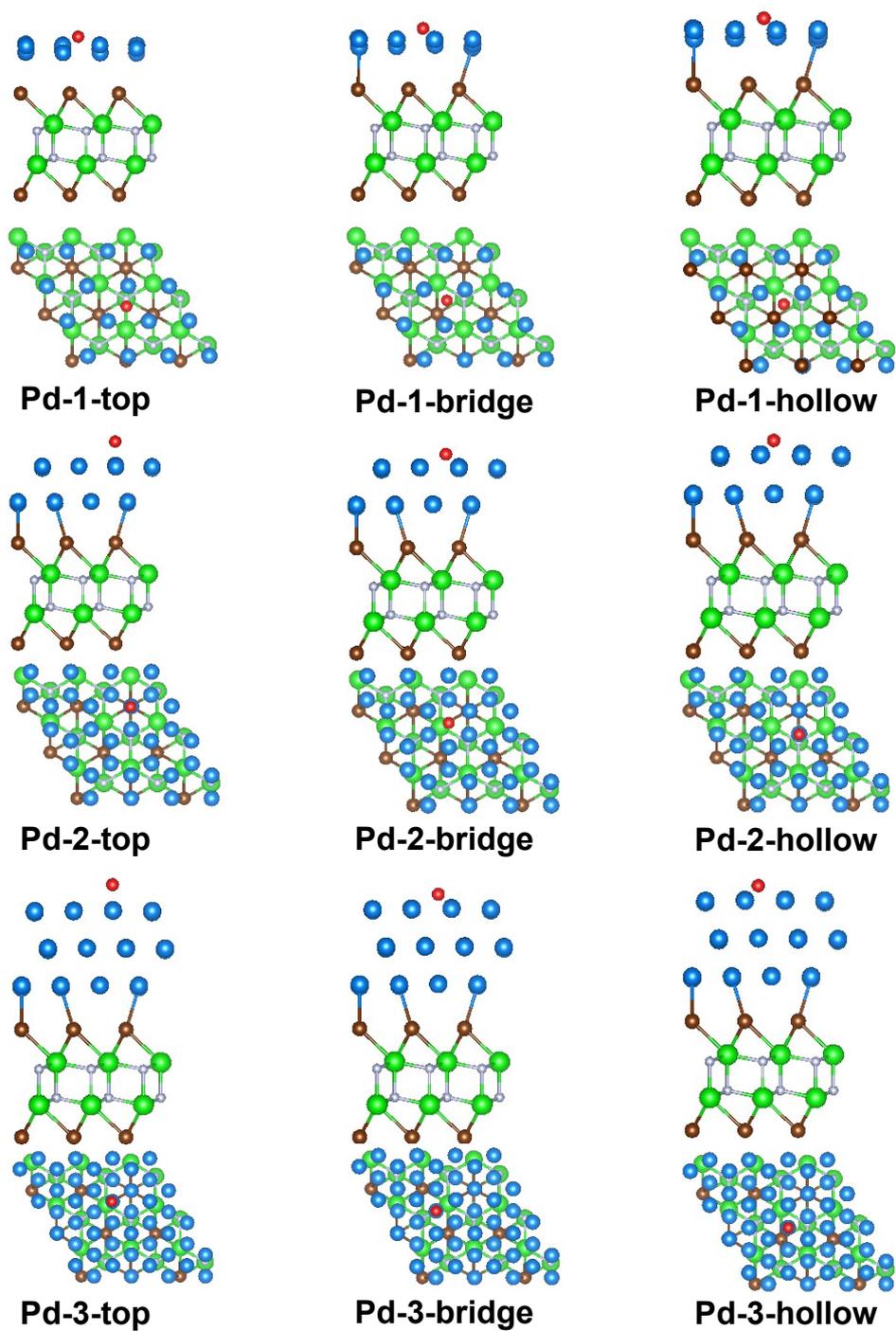


Fig. S4 Side and top views of the optimized structures for H adsorbed Pd/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), blue (Pd), and red (H).

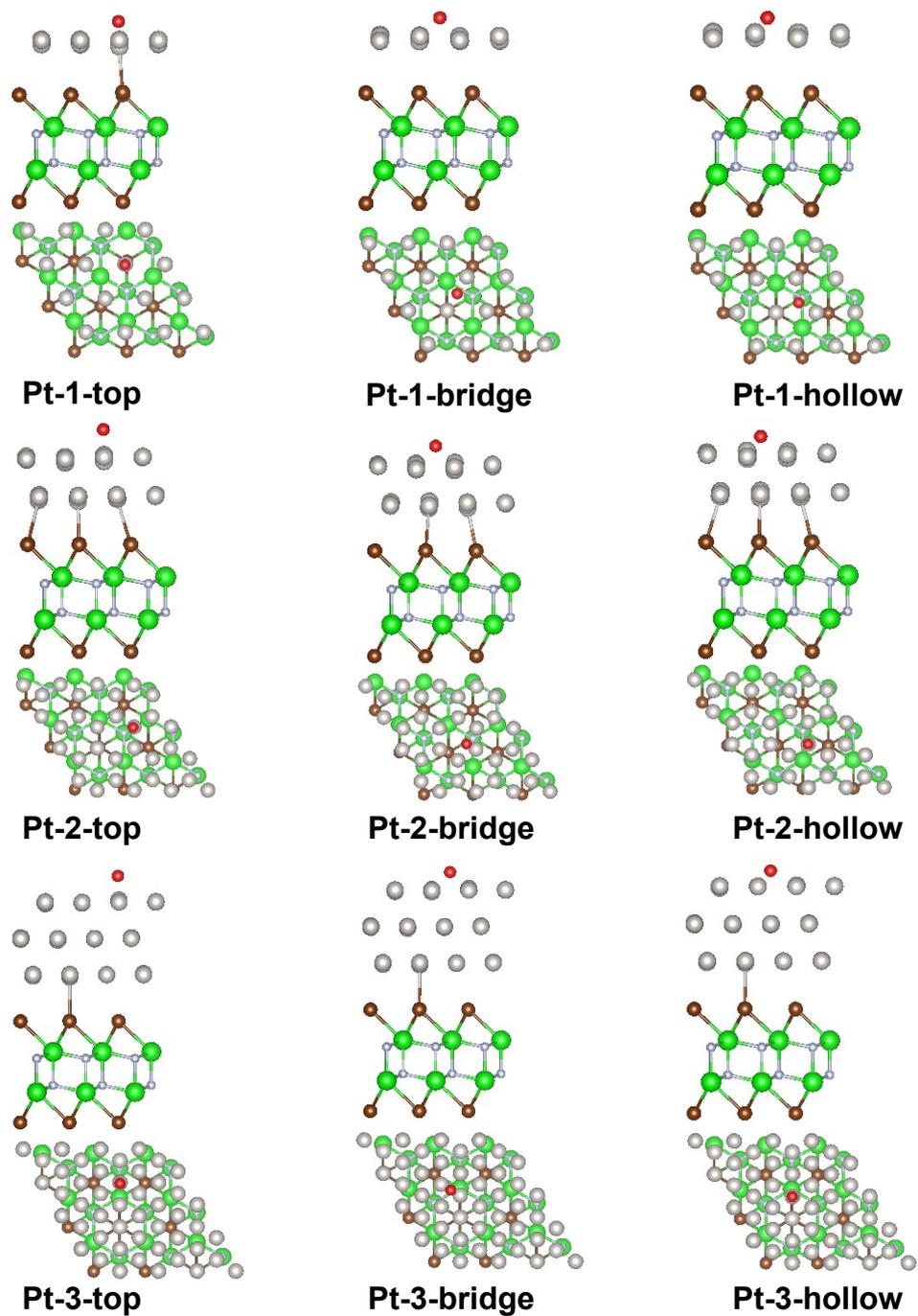


Fig. S5 Side and top views of the optimized structures for H adsorbed Pt/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), silver (Pt), and red (H).

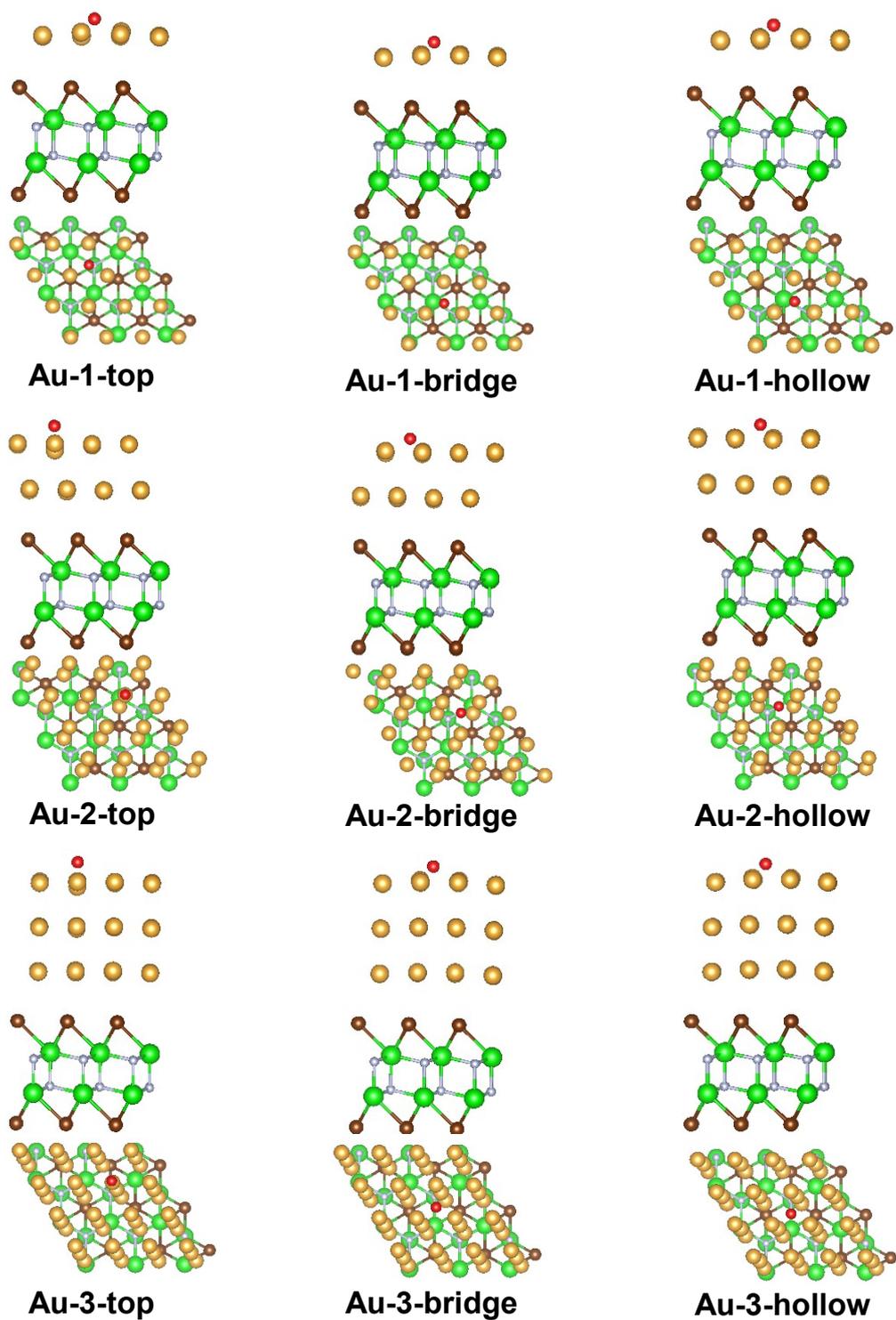


Fig. S6 Side and top views of the optimized structures for H adsorbed Au/ZrNBr heterostructures. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), yellow (Pt), and red (H).

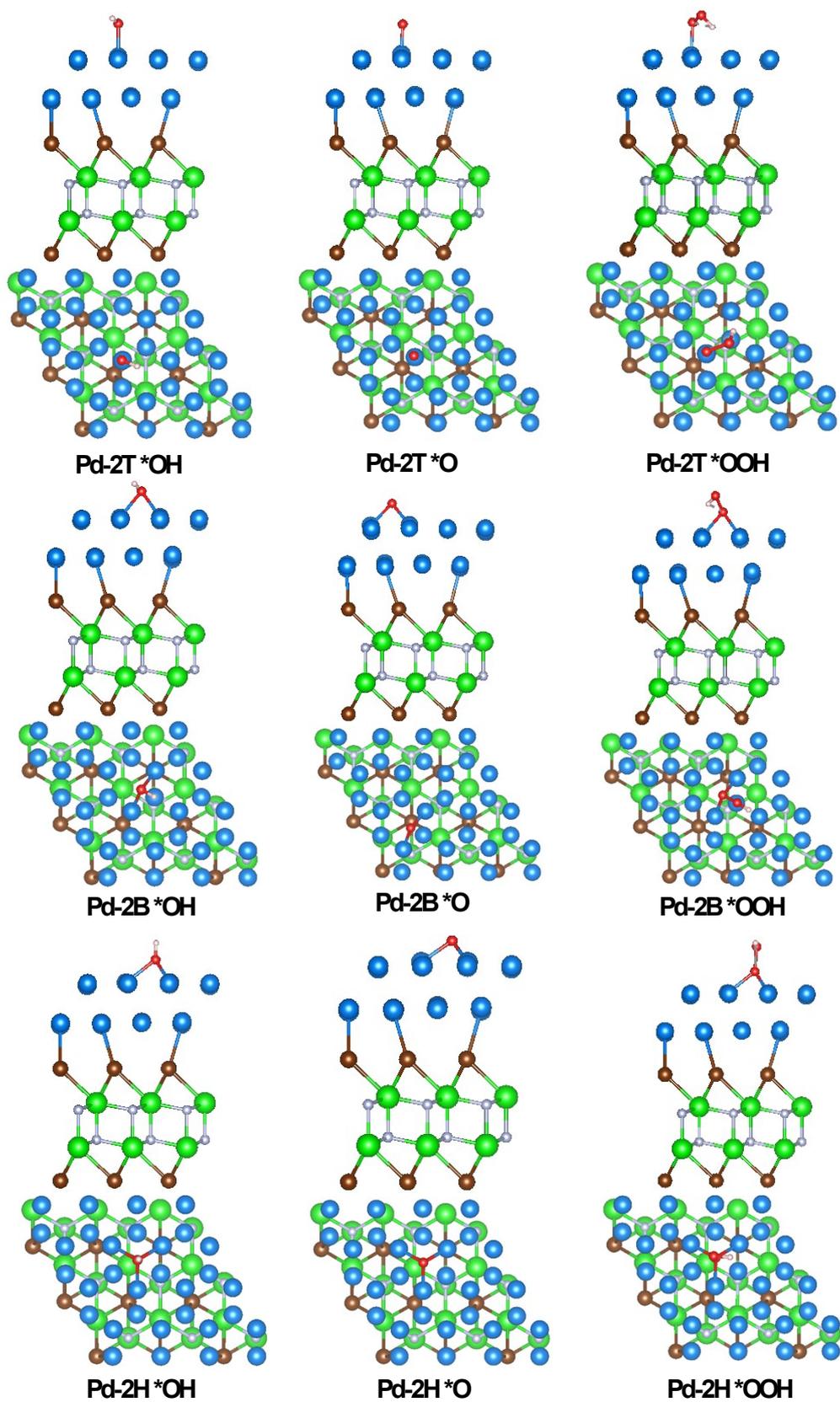


Fig. S7 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Pd-2T**, **Pd-2B** and **Pd-2H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), blue (Pd), red (O), and white (H).

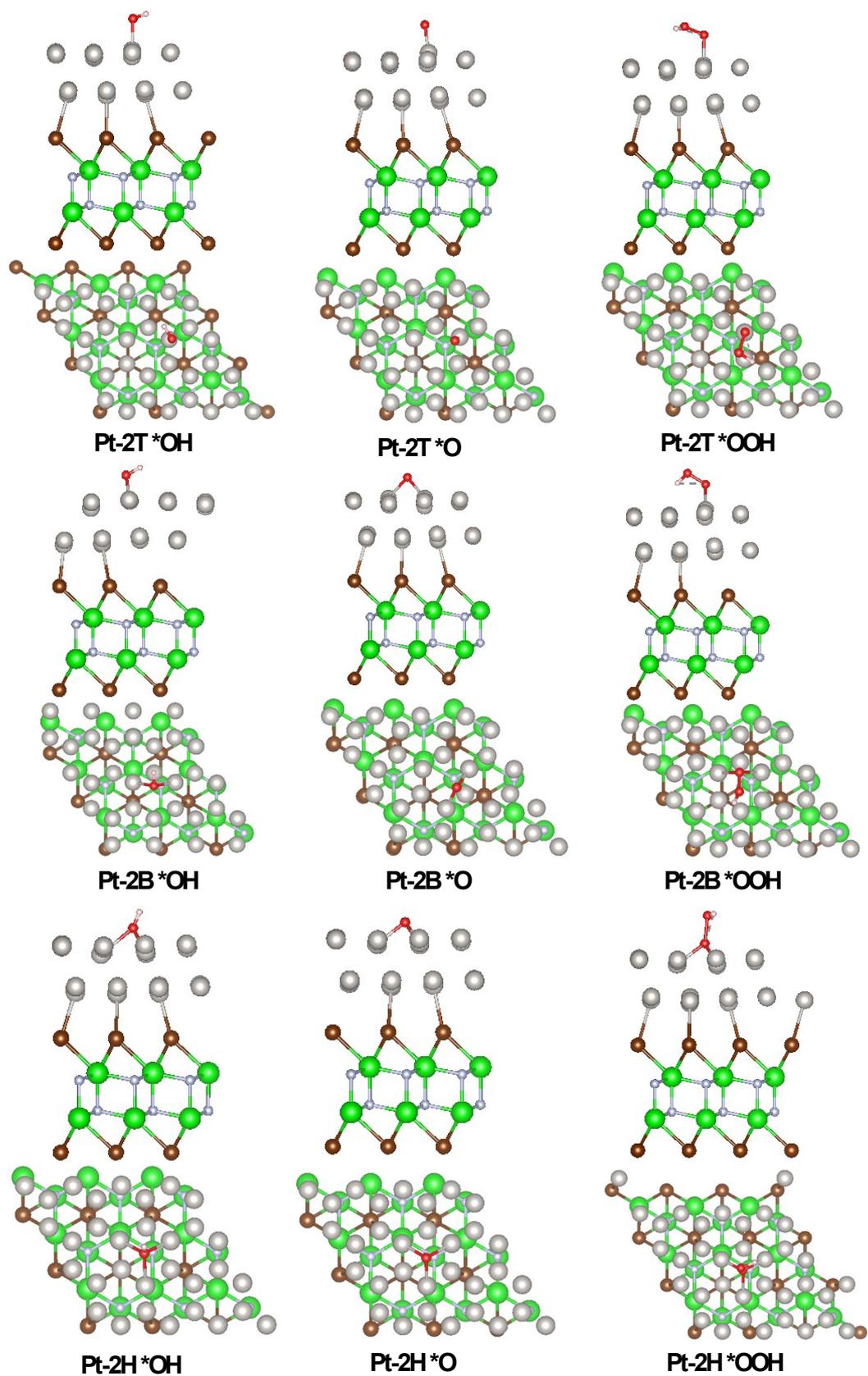


Fig. S8 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Pt-2T**, **Pt-2B** and **Pt-2H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), silver (Pt), red (O), and white (H).

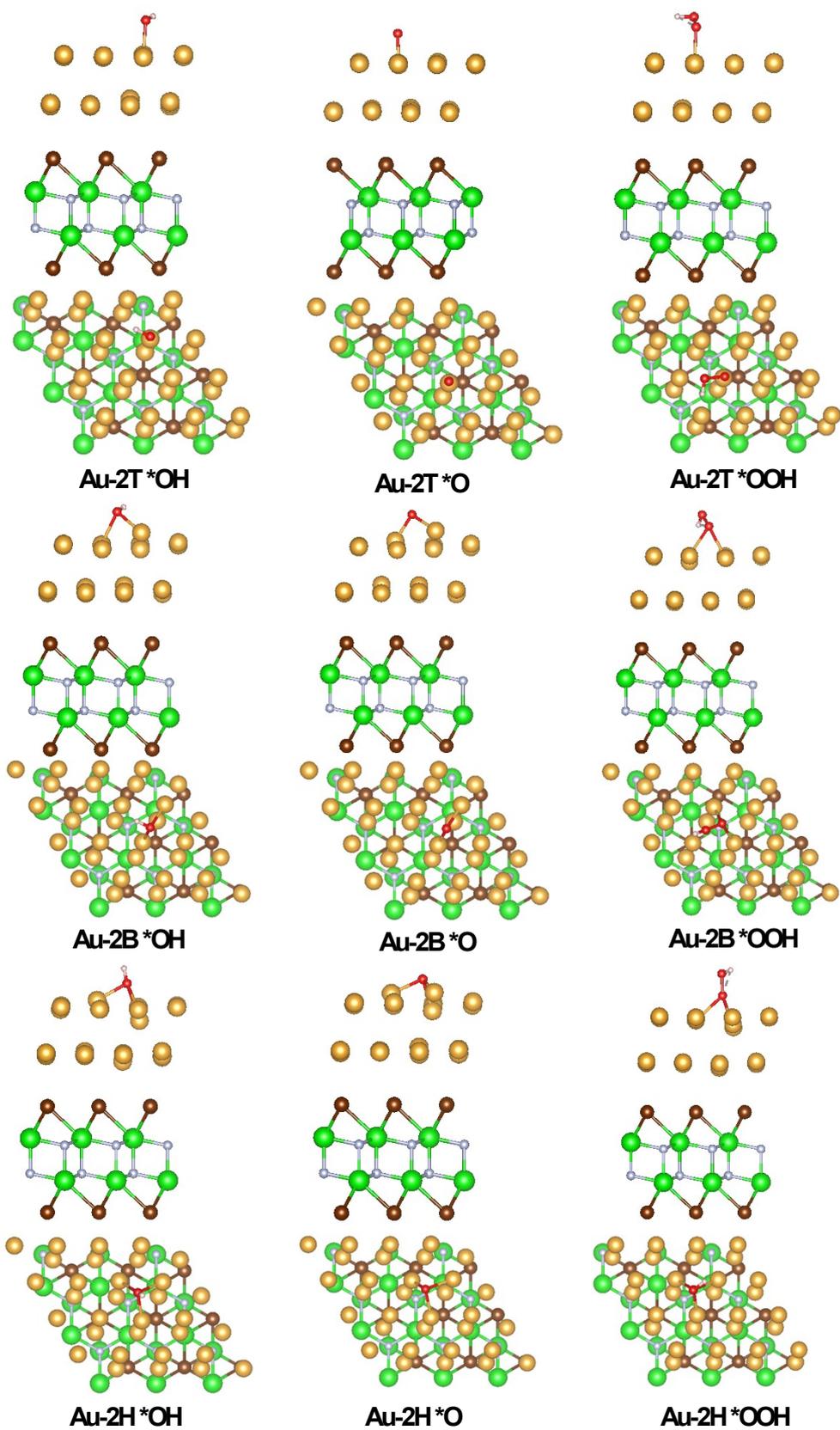


Fig. S9 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Au-2T**, **Au-2B** and **Au-2H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), yellow (Au), red (O), and white (H).

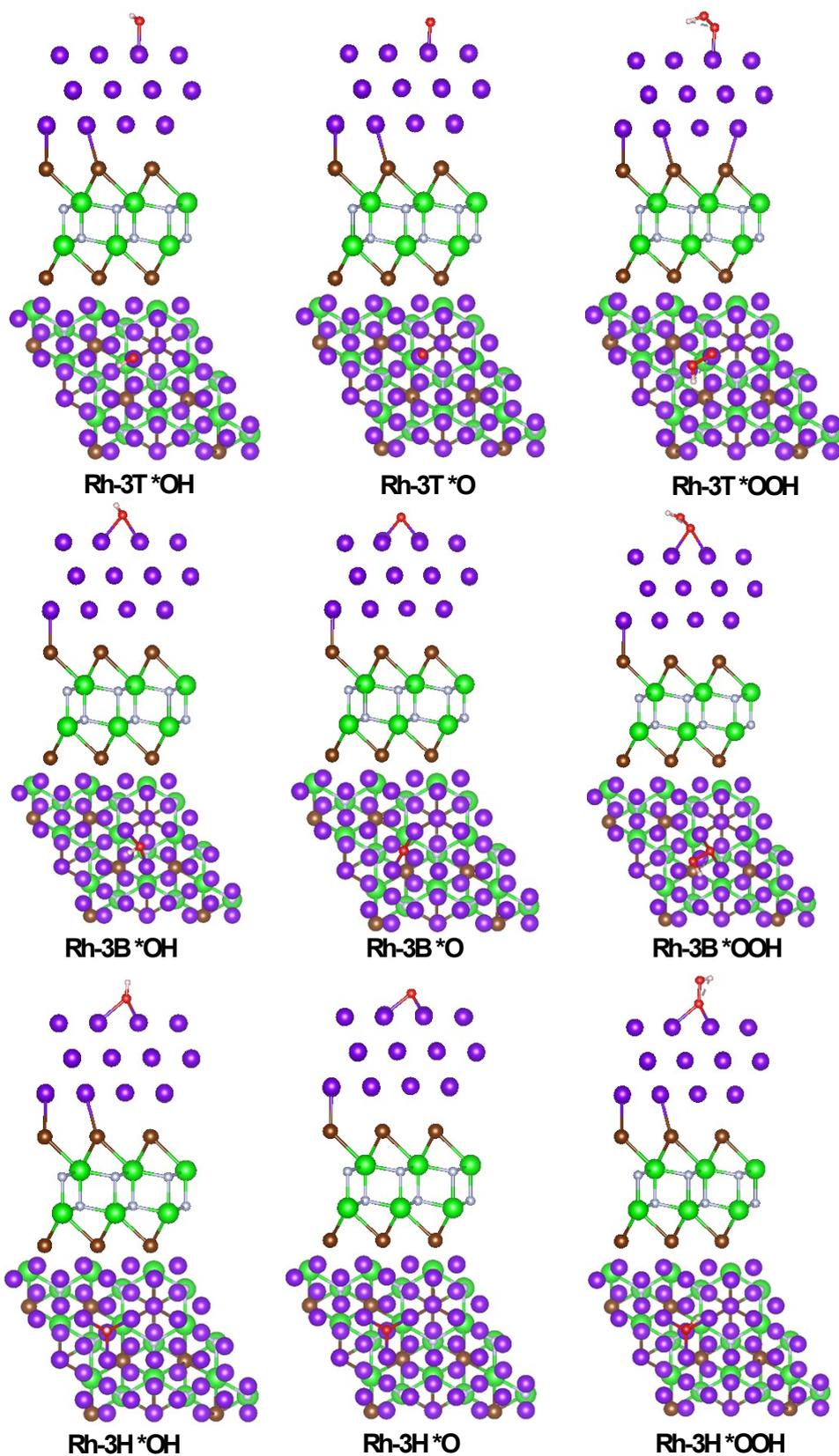


Fig. S10 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Rh-3T**, **Rh-3B** and **Rh-3H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), purple (Rh), red (O), and white (H).

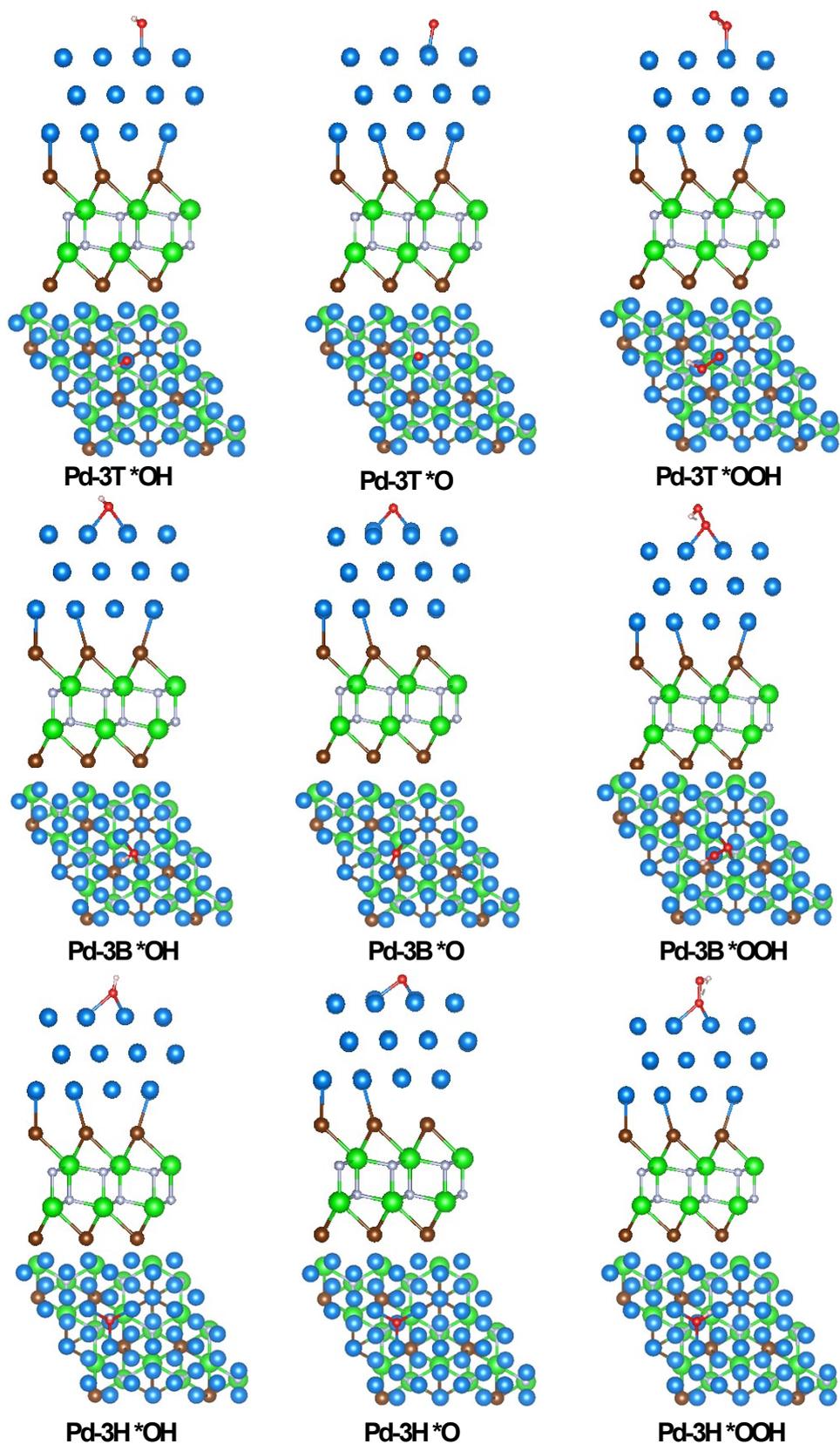


Fig. S11 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Pd-3T**, **Pd-3B** and **Pd-3H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), blue (Pd), red (O), and white (H).

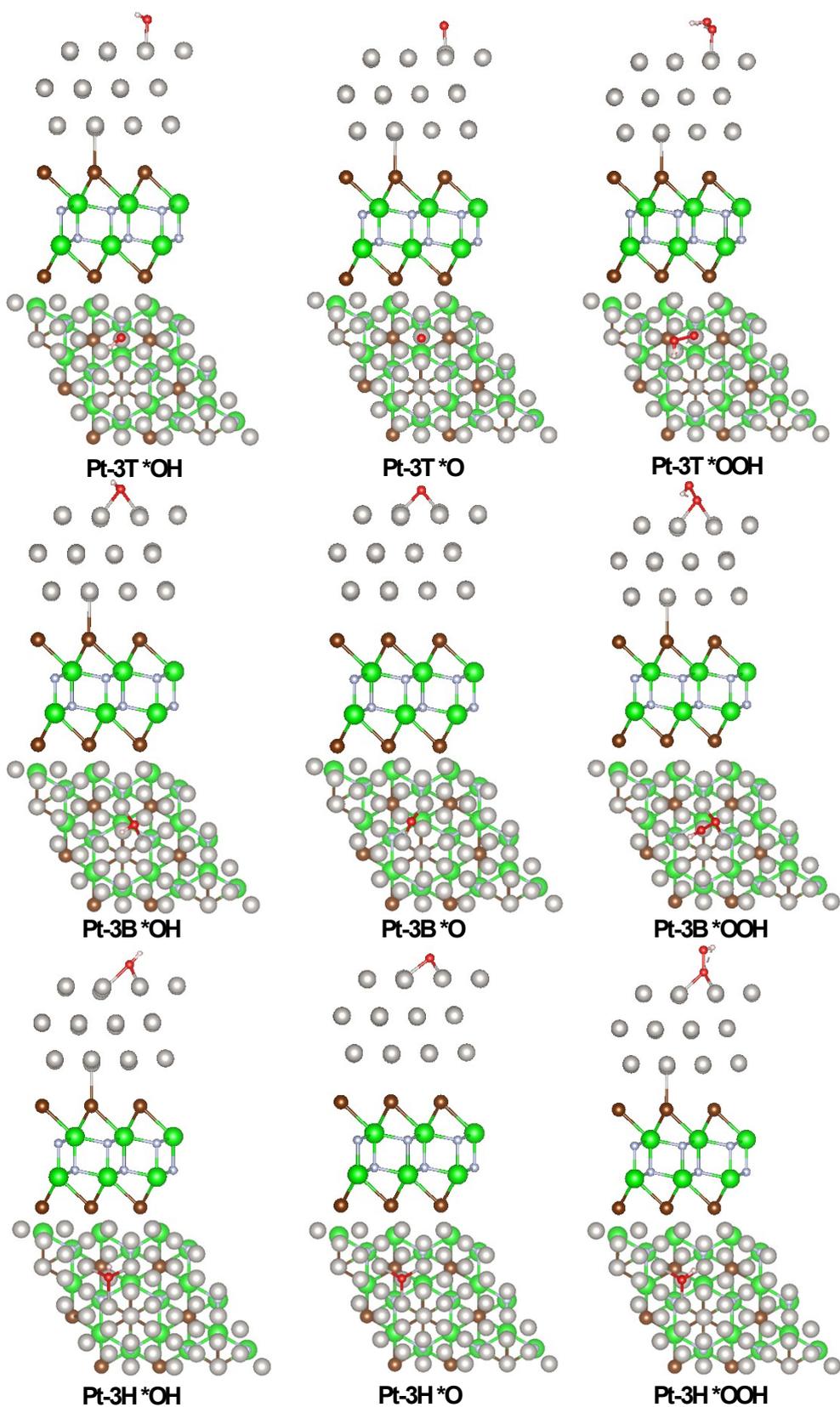


Fig. S12 Optimized structures of *OH, *O and *OOH intermediates for the OER on **Pt-3T**, **Pt-3B** and **Pt-3H**. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), silver (Pt), red (O), and white (H).

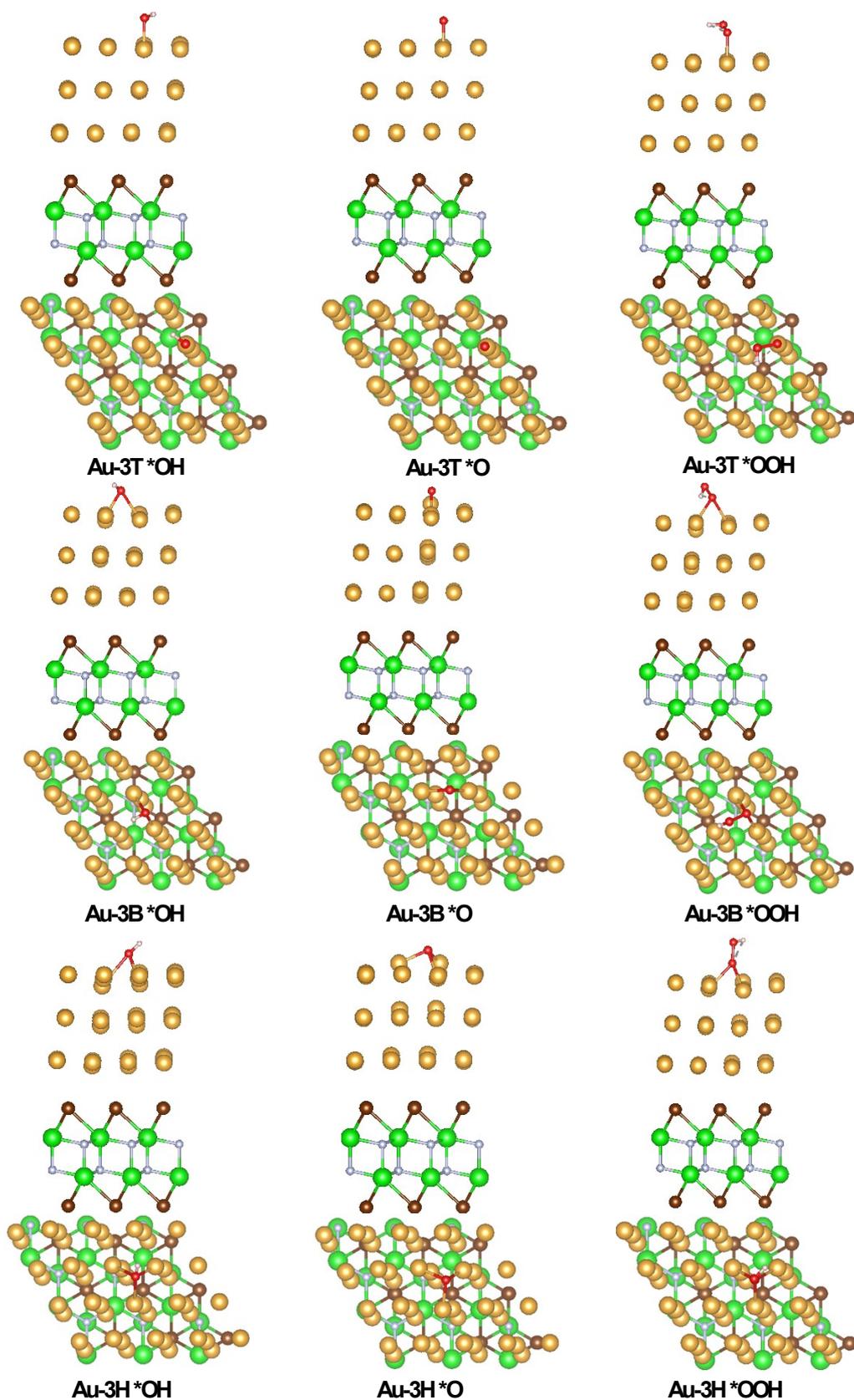


Fig. S13 Optimized structures of $*OH$, $*O$ and $*OOH$ intermediates for the OER on Au-3T, Au-3B and Au-3H. Coloring scheme of atoms: green (Zr), lilac (N), brown (Br), yellow (Au), red (O), and white (H).