

EIS: Electronic Supplementary Information:

Followings equations show the energy of reaction and energy of oxygen vacancy formation in reduction reactions of metal oxide with H₂, that creates H₂O and metal oxide with one added oxygen vacancy.

It shows that the difference in the formation energy of first and second oxygen vacancy is equal to the difference between the energy of first and second reaction.

$$E_{r1} = E_{Ovacancy\ System} + E_{H_2O} - E_{H_2} - E_{fullsystem}$$

$$E_{r2} = E_{2Ovacancy\ System} + E_{H_2O} - E_{H_2} - E_{Ovacancy\ System}$$

$$Del - E = E_{2Ovacancy\ System} + E_{H_2O} - E_{H_2} - E_{Ovacancy\ System} - (E_{Ovacancy\ System} + E_{H_2O} - E_{H_2} - E_{fullsystem})$$

$$Del - E = E_{2Ovacancy\ System} + E_{H_2O} - E_{H_2} - E_{Ovacancy\ System} - E_{Ovacancy\ System} - E_{H_2O} + E_{H_2} + E_{fullsystem} =$$

$$Del - E = E_{2Ovacancy\ System} - E_{Ovacancy\ System} - E_{Ovacancy\ System} + E_{fullsystem}$$

$$E_{v1} = E_{Ovacancy\ system} + \frac{1}{2}E_{O_2} - E_{full\ system}$$

$$E_{v2} = E_{Ovacancy\ system2} + \frac{1}{2}E_{O_2} - E_{Ovacancy\ system}$$

$$Del - E_v = E_{Ovacancy\ system2} + \frac{1}{2}E_{O_2} - E_{Ovacancy\ system} - (E_{Ovacancy\ system} + \frac{1}{2}E_{O_2} - E_{full\ system})$$

$$Del - E_v = E_{Ovacancy\ system2} - E_{Ovacancy\ system} - E_{Ovacancy\ system} + E_{full\ system}$$

$$Del - E_v = Del - E$$

E_{r1} represents energy of first reaction which results in creation of one oxygen vacancy ($E_{Ovacancy\ System}$).

$E_{fullsystem}$ represents the energy of reactant in first reaction.

$E_{Ovacancy\ System}$ represents the energy of product in first reaction.

E_{r2} represents energy of second reaction which results in creation of two oxygen vacancies.

$E_{2Ovacancy\ System}$ represents the energy of product in the second reaction.

$Del - E$ represents the difference between the energy of first and second reaction.

E_{v1} formation energy of the first oxygen vacancy.

E_{v2} formation energy of the second oxygen vacancy.

$Del - E_v$ represents the difference between the formation energy of first and second oxygen vacancy.