Oxygen Reduction on Transition Metal Chalcogenides

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Abstract & Objectives

Fuel cells are of great interest, because they are a key element of the emerging hydrogen economy. One of the most promising types of fuel cells is the Proton Exchange Membrane Fuel Cell (PEMFC), because it is A highly efficient power and a prime candidate for variety applications of vehicles. The biggest obstacles in PEMFC`s commercialization are cost and lifetime. Therefore, searching for new electrocatalytic materials with a reduced loading of precious metals with significant improvement of the electrocatalytic properties of the electrodes is critical for commercialization of PEMFC. To reach this goal, a density functional theory (DFT) calculations are performed to study the oxygen reduction reaction on selenium and sulfur-containing transition metal Surfaces and the effect of the chalcogen on the activity, selectivity and stability of the catalyst is investigated.

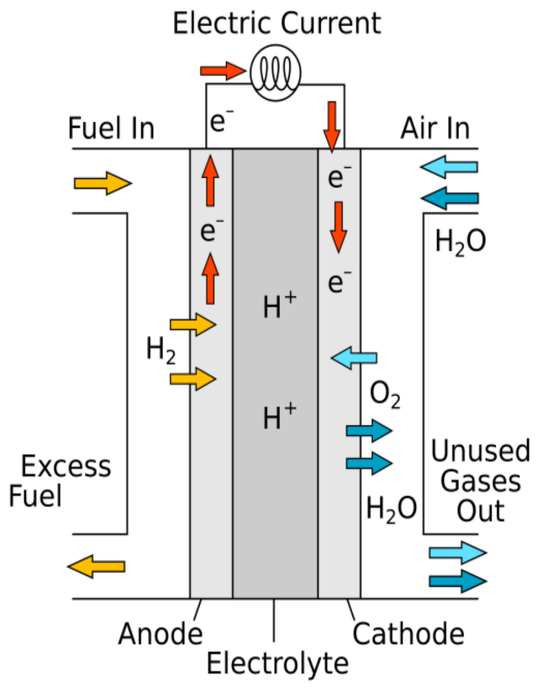


Fig.1: PEMFC schematic

Materials & Methods

The calculations are carried out within DFT using the plane wave basis set and pseudo-potential method as embodied in the code PWSCF with ultra-soft. A super-cell geometry is used to simulate the surface, see Fig (2). The adsorbents are allowed to reach the surface only on one side of the slab.

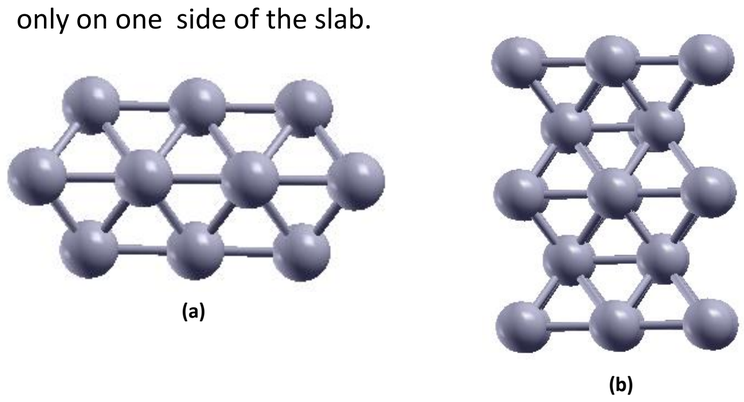


Fig.2: a is 3×2 super-cell and b is 2×2 super-cell.

The adsorption of the adsorbents is examined at high symmetry.
sites (top, hollow, bridge) for each coverage, see Fig.3.

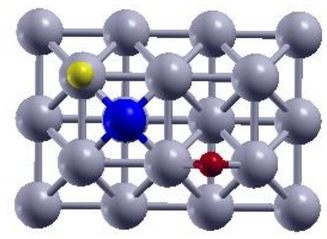
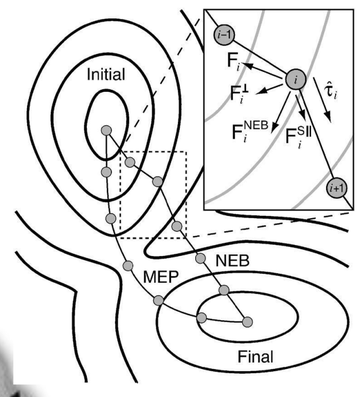


Fig.3: The high symmetry sites: yellow for top, blue for hollow and red for bridge



The reaction path and barrier are searched for by using Nudge elastic band method ., see Fig.4.

Fig.4: The Nudge Elastic Band method.

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Results (still working)

A. The adsorption of S (or Se) on Ir(100) surface

The adsorption of S (or Se) atom on Ir(100) surface with different coverages is investigated. The hollow site is found to be the most energetic stable adsorption site for both adsorbents.

B. The co-adsorption of S (or Se) with O atom and O_2 molecule on Ir(100) surface

Oxygen atom prefers the bridge site when adsorbed on Ir(100) surface with adsorption energy 5.20 eV. However, O_2 molecule adsorbed weakly on Ir(100) surface when it reaches it vertically with adsorption energies less than 1 eV. The effect of the co-adsorption of S (or Se) with O and O_2 on Ir(100) surface is investigated and the calculations are still working, see Fig. 5.

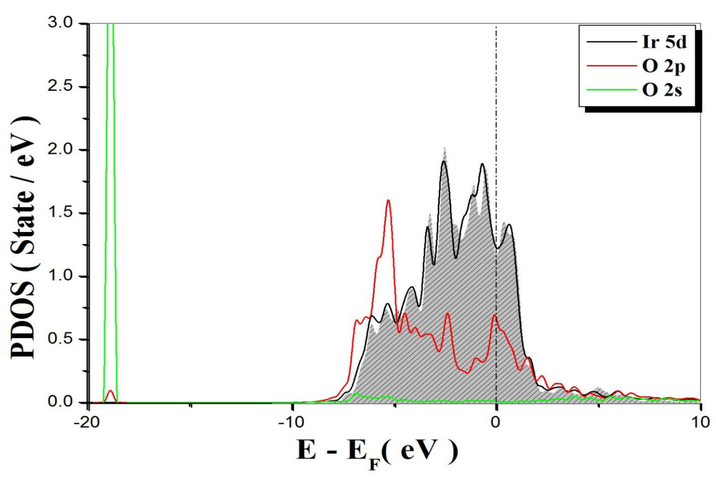
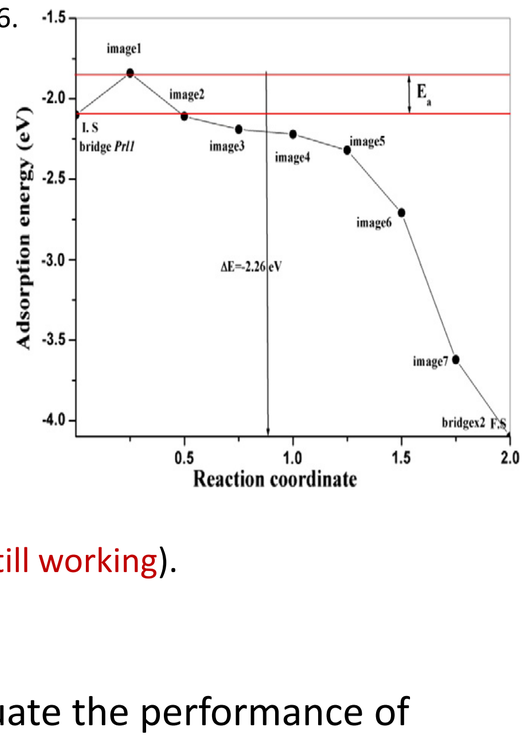


Fig. 5. The PDOS of O/Ir(100) system, the solid line denotes Ir 5*d* *band for the first Ir layer in O/Ir (100) system and the shadow denotes the 5d band of the clean Ir(100) surface.*

The dissociation of O_2 molecule on Ir(100)-S (or Se) surface

The dissociation of O_2 on Ir(1 0 0) surface was studied previously by Erikat et. al and a small barrier (0.26 eV/O_2)is found, see Fig. 6.



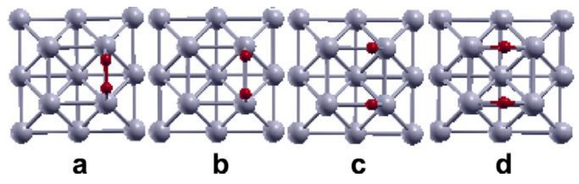


Fig.6: Selected states along the path of O_2 dissociation on Ir(100) surface and the reaction minimum energy path. Erikat (2011)
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The same reaction will be done by using NEB Method on Ir(100)-S (or Se) surface (Still working).

Conclusion

DFT calculations is performed to evaluate the performance of transition metal surfaces modified with S or Se as cathode catalysts for low-temperature fuel cells. The effect of the chalcogen on the activity, selectivity and stability of the chalcogen-containing surface is studied by adsorbing S and Se on Ir(100) surface different coverages. The activity for oxygen reduction reaction on transition metal chalcogenide surfaces is estimated.

References

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