# Computational Modelling of Thermoelectricity, Carrier Mobility and Electro-Catalytic Oxygen Reduction Reaction: a Few Examples

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**Abstract:** In recent years, many van der Waals solids, perovskites, spinels etc. exhibit many fold benefits for applications in a number of fields, namely, transparent substrates, field effect transistors, solar cells, thermoelectric materials, active surface for catalysis, rechargeable battery etc, to name a few. In fact, recent experimental advancements on the control over the surface structure of materials has enabled material scientists to tailor the material properties with improved reliability and functionality. We have derived relaxation time formulation from complete Boltzmann transport equation and obtained all the parameters from ab-initio density functional theory. Using this formalism, we have calculated charge carrier mobility values and important descriptors. A few cases, such as, trilayer phosphorene and bilayer $MoS_2$ polytypes will be discussed [1]. We have also been working on Carbon dioxide reduction, Oxygen evolution and reduction reaction by finding stable, cheap and active catalytic surfaces. In this context, I shall discuss the oxygen evolution reaction (OER) on pure and metal doped cobalt oxides, $Co_3O_4$ and $MxCo_3$-$xO_4$, (M = Fe, Ni, Cu) surfaces in acidic media, where the substantial work has been targeted to understand the relation between structure, mechanism, and activity. The activity of the substituted spinels increases relative to that of pure $Co_3O_4$ and we find that 25% substitution of Cu in $Co_3O_4$ has highest electro-catalytic activity in acidic media with a reduced over-potential value of 0.41 V for OER [2]. Further, in basic media, we have carried out OER on oxygen deficient pristine and doped double perovskite, $Ca_2Mn_2O_5$, where Ca is replaced with inexpensive alkaline earths, main group elements, and lanthanides to elucidate how the electronic structure can aptly be tuned by doping, for the best catalytic performance [2]. We have also worked out in detail the thermoelectric behavior of SnTeSeS systems by co-doping with Ag and In and found the microscopic reason for thermoelectric efficiency to be 1.3 in the case of one of the composition of AgInSnTeSeS. If time permits, I shall also discuss developing anodic material for Mg-ion rechargeable battery [3].

## References

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