LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

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Outline

- Cr based alloy Cr-Y oxidation study
- High temperature oxidation of Y doped Nb_2AlC study
- Simulation on GR-H-SiO_2 system
- Simulation on CNTs with Nitrogen doped
- Tools
- Acknowledgement

Study on Cr-Y system

Introduction:

1. Chromium(Cr)

- High melting point (1907°C)
- Low density
- Good high temperature strength
- Easily oxidized at a high temperature above 800°C

2. Benefits of Cr based alloys

The doping of transition metals such as Y, Ce and La in Cr-based alloys can reduce the residual oxygen content in the bulk by forming very stable oxides to enhance extrinsic ductility. The slow diffusivities of these dopants and dispersion strengthened oxides increase the creep resistance of Cr-based alloys.

Study on Cr-Y system

Computation Method:

1. In this work, we studied the properties of bulk Cr with Y doping at high temperatures using ab Initio molecule dynamic (MD) DFT method.

- Different densities of Y-doping (Y/Cr): 2.46%, 5.04%, 13.64%.
- Different temperature: 1200K ~ 2100K

2. A cubic supercell consisting of 250 chromium atoms is set as 5×5×5 (repeating original Cr unit cell 5 times in X, Y and Z directions). Y atoms are randomly dispersed to Cr bulk. (Figure 1)

3. To study oxidation progress of Cr-Y alloys at high temperatures, two layers of oxygen atoms are put at the top and bottom of Cr-Y surfaces respectively. (Figure 2)

Study on Cr-Y system

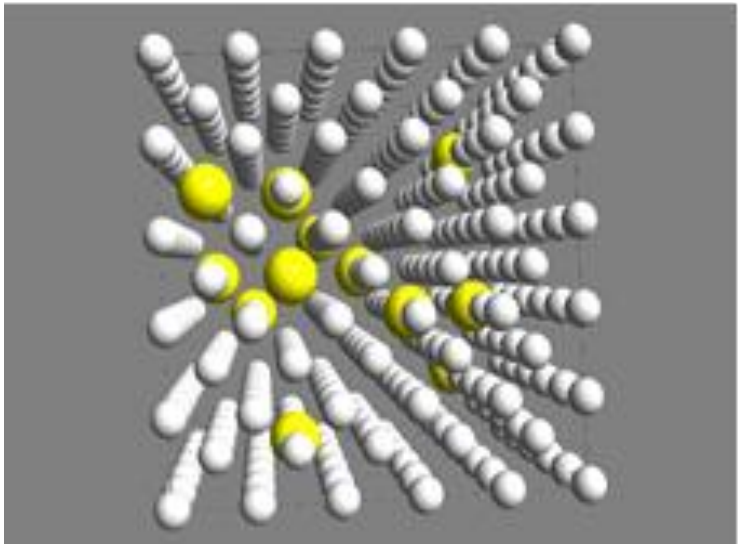


Figure 1. Cr with Y doping system at initio state. 238 Cr atoms (White) and 12 Y atoms (Yellow) are shown in the figure.

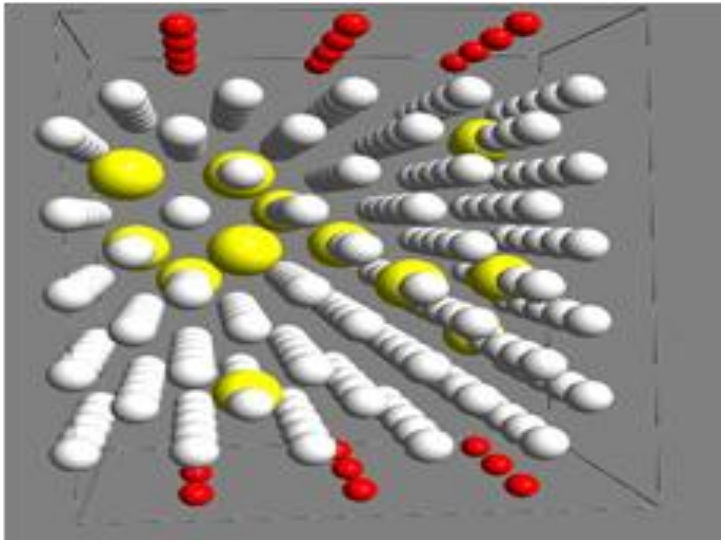


Figure 2. O/Cr-Y alloy system at initio state. 238 Cr atoms (White), 12 Y atoms (Yellow), and 21 O atoms (Red) are shown in the figure.

Study on Cr-Y system

Computation Method:

4. Preforming DFT MD Simulations

5. Using local-density approximation (LDA) method with ultrasoft pseudopotentials, representing the ionic core effect

6. The simulation is based on Vienna Ab Initio Simulation Package (VASP) with NVT ensemble.

Study on Cr-Y system

Result and Discussion:

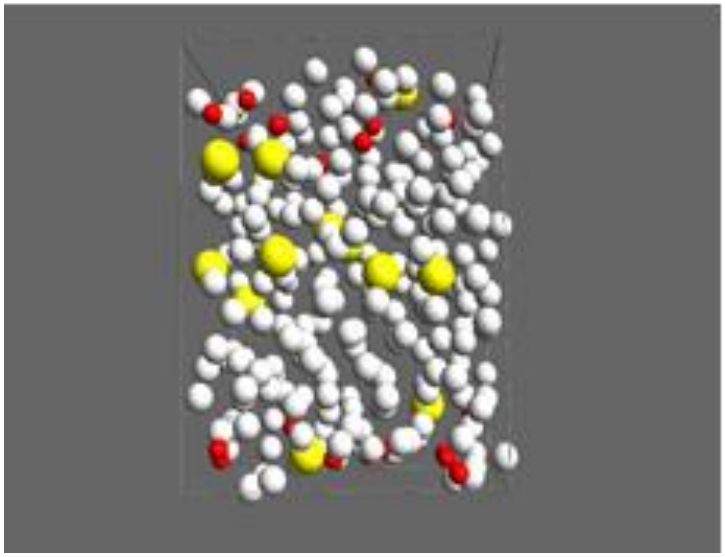
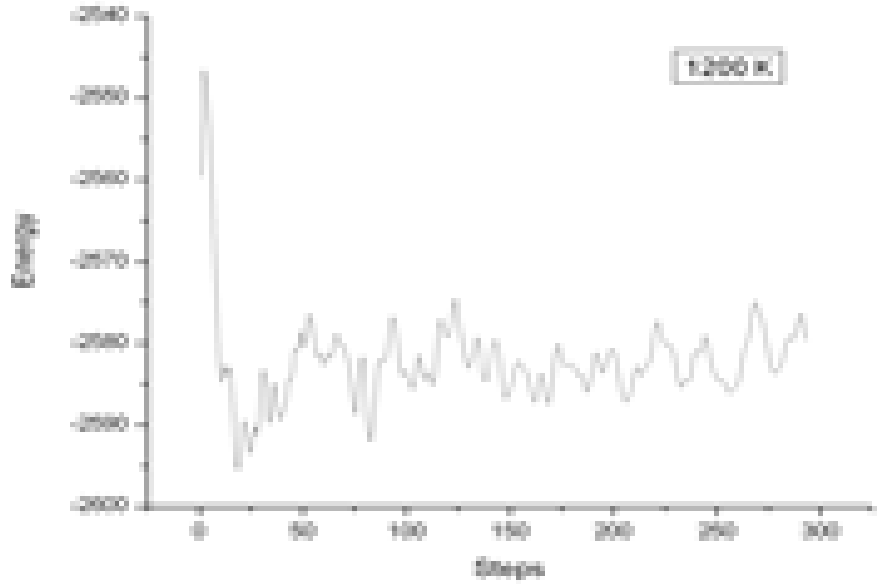


Figure 3. O/Cr-Y system at 1200 K with O atoms diffused. 238 Cr atoms (White), 12 Y atoms (Yellow), and 21 O atoms (Red) are shown in the figure.

Figure 3 shows that at T=1200K, after about 1 ps MD run, the O/Cr-Y final configurations. We found from our 1200K ~ 2100K Cr-Y alloy simulation that the Cr-Y lattice is stable up to about 1800K. From the simulation results, we can clearly see that Y doping enhances oxidation resistance of Cr alloys

Study on Cr-Y system

Result and Discussion:



The energy convergence with run time at T=1200K is shown in Figure 4 (The energy unit is in eV).

Figure 4. Energy at every step vs. time steps in the MD simulation.

Study on Cr-Y system

Result and Discussion:

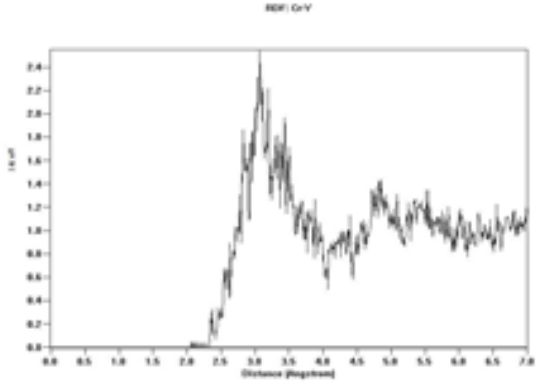


Figure 5. RDF of Cr-Y

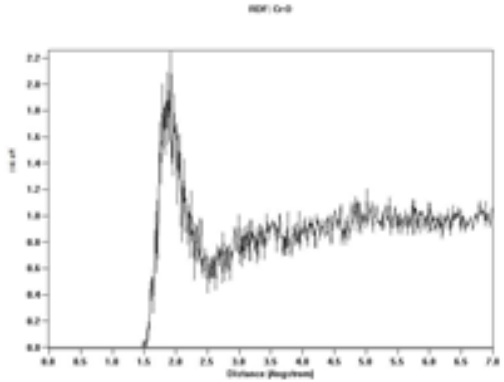


Figure 6. RDF of Cr-O

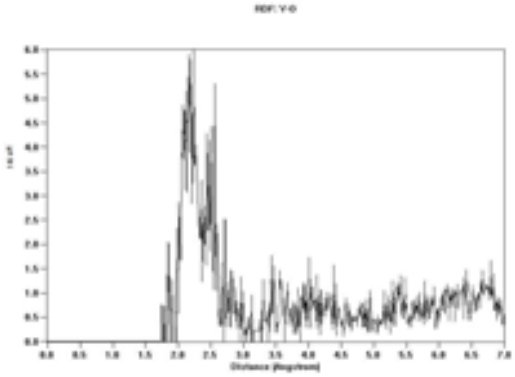


Figure 7. RDF of Y-O

Figs. 5~7 displayed the radial distribution function (RDF) of Cr-Y, Cr-O, and Y-O respectively. Figs. 5 ~ 7 show that the Cr-Y main distance is at 3.2 Å, the Cr-O main bond length is at 1.9 Å and Y-O main bond length is at 2.2 Å. Also we can see that Y-O bond distribution peak is sharp show strong interactions between Y and O atoms.

Study on Cr-Y system

Drawback:

It is necessary to mention that our simulation is only limited to 1ps MD time, this can also be seen from the small fluctuation of the energy ~ simulation step curve. To get the final stable structure of the oxidized Cr-Y alloy, more simulation time steps are needed.

Study on Cr-Y system

Conclusion:

We have performed *ab initio* MD simulation on the stability and oxidation of Cr-Y alloy. The results show that Y doping enhanced the oxidation resistance capability of Cr-based alloy by forming strong Y-O bonds. Appropriate refractory transition metal components co-doping may needed in designing Cr-based alloy for high temperature applications.

Study on Nb2AlC-Y system

Introduction:

1. Niobium (Nb)

- high melting temperature (2469°C)
- mediate density (8.6 g/cm3)
- high thermal conductivity
- Has potential application in many high temperature applications

2. Nb-based alloys

- Nb-based alloys have a poor oxidation resistance at high temperature (>600 °C) and thus a high quality thermal barrier coating (TBC) is necessary for stable long term application.
- Y doping
- Mo doping

Study on Nb2AlC-Y system

Computation Method:

1. In this work, we studied the properties of bulk Nb2AlC with Y and Y-Mo co-doping at high temperatures using ab initio molecule dynamic DFT method.

- Temperatures: 1200K~2100K

2. Supercell: 4×4×2 (128 Nb atoms, 64 Al atoms, 64 C atoms) unit cell (Figure 8). For Y and Mo doping, the 10 Nb atoms are randomly replaced by Y and Mo atoms (Figure 9).
3. Oxygen atoms were then added at both ends of the supercell (Figure 10).
4. Preforming DFT MD Simulations
5. LDA
6. Main Package: VASP with NVT ensemble

Study on Nb2AlC-Y system

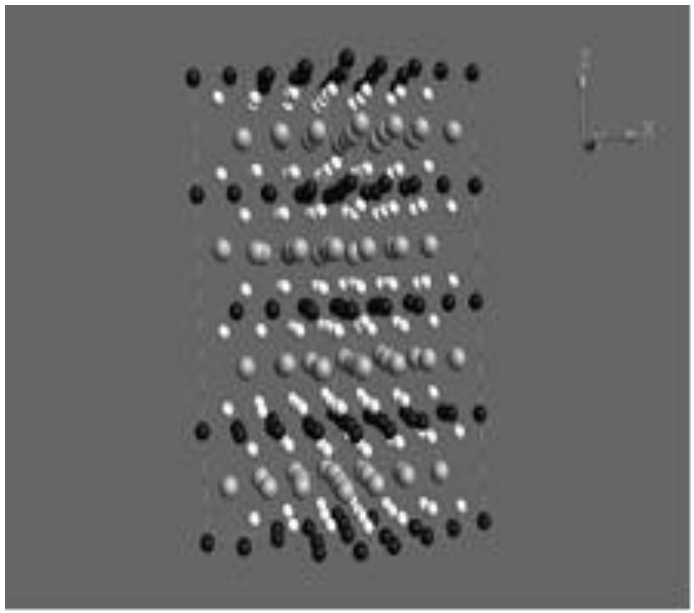


Figure 8. Nb_2AlC system. There are 128 Nb atoms (White), 64 Al atoms (gray), 64 C atoms (Black) in the supercell.

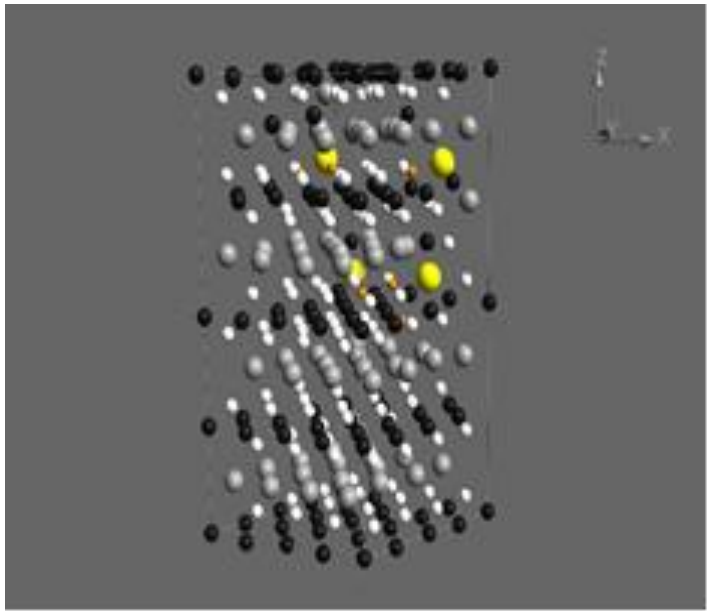


Figure 9. Y and Mo co-doped Nb2AlC system. There are 118 Nb atoms (White), 64 Al atoms(gray), 64 C atoms (Black), 6 Mo atoms(Orange), and 4 Y atoms(Yellow)in the supercell.

Study on Nb2AlC-Y system

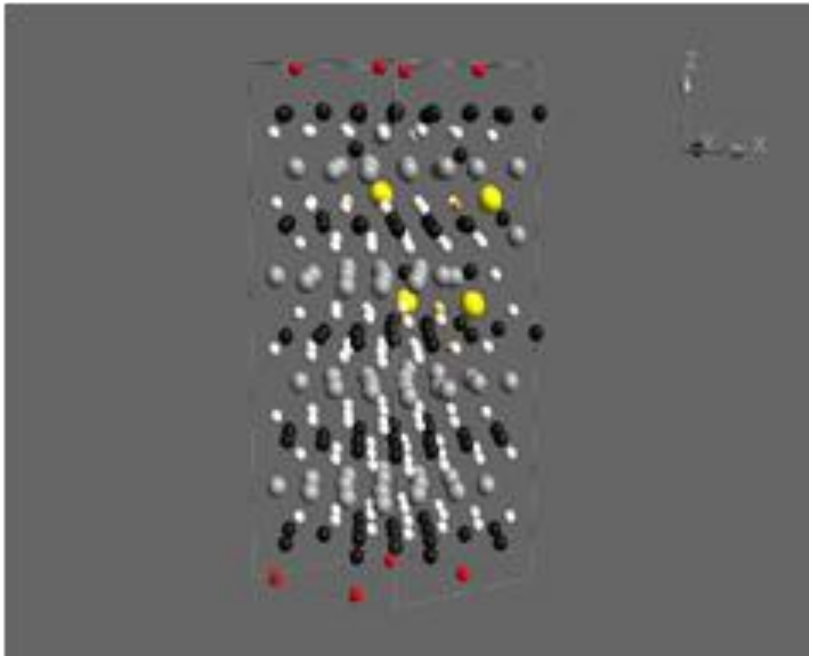


Figure 10. Y and Mo co-doped Nb2AlC system. There are 118 Nb atoms (White), 64 Al atoms(gray), 64 C atoms (Black), 6 Mo atoms(Orange), 4 Y atoms(Yellow) and 8 O atoms(Red)in the supercell.

Study on Nb2AlC-Y system

Result and Discussion:

- Nb_2AlC lattice is stable up to about 2100K.
- When Y atoms are doped into Nb layer, the nearby C and Al atoms in the C and Al layers are fluctuated and jump out the layers forming local defects.
- The MD trajectory shows that the Mo atoms doping enhanced the layered structure.
- From the simulation results, we can clearly see that Y doping enhances oxidation resistance of Cr alloys.
- Y and Mo doping improves the stability of high temperature mechanical property and blocks the O diffusion path.

Study on Nb2AlC-Y system

Conclusion:

We have performed ab initio MD simulation on the oxidation of Y and Mo co-doped Nb_2AlC MAX phase structure. The results show that Y and Mo doping enhanced the oxidation resistance capability of the Nb_2AlC by forming strong Al-O and Y-O bonds. The doping also enhances the inter-layer bonding and thus the high temperature mechanical property and thus has potential application in Nb-based alloy coating. Appropriate refractory transition metal components co-doping may be needed in designing the MAX phase Nb_2AlC for high temperature applications.

Simulation on GR-H-SiO_2 system

Graphene, a truly two dimensional material with carbon honey comb plane structure has attracted tremendous attention since its first realization in 2004, largely due to its unique electronic properties that makes graphene a promising candidate to replace silicon in next generation of semiconductor devices and sensing applications .

Simulation on GR-H-SiO_2 system

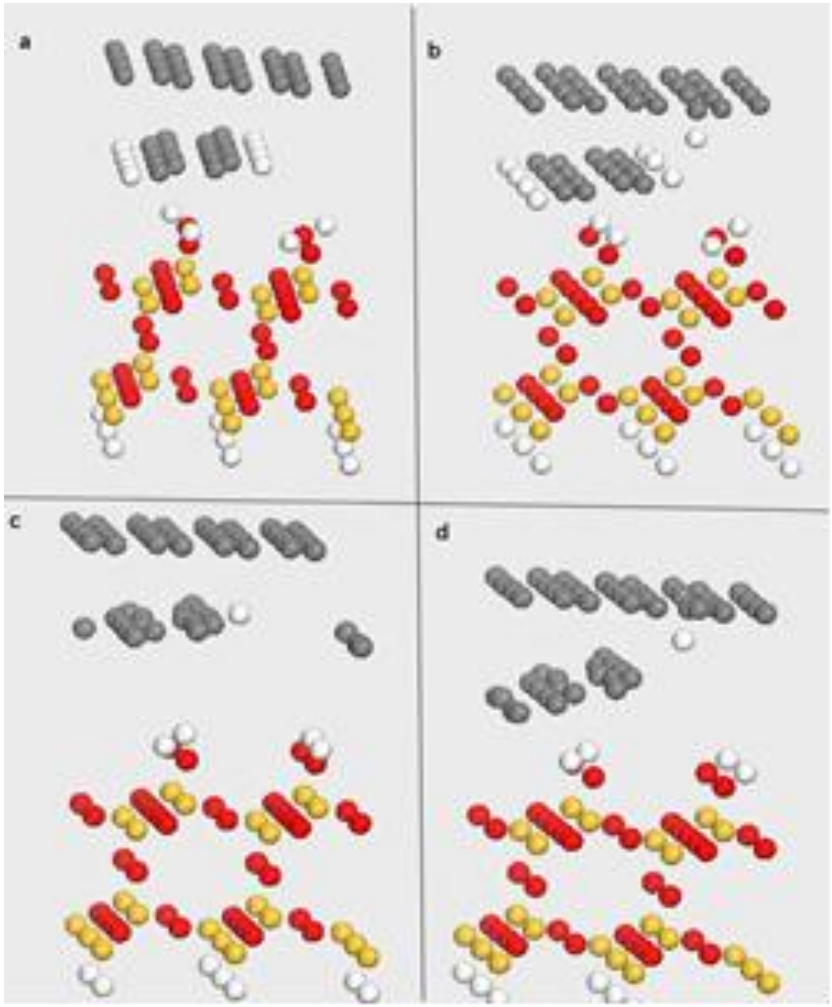
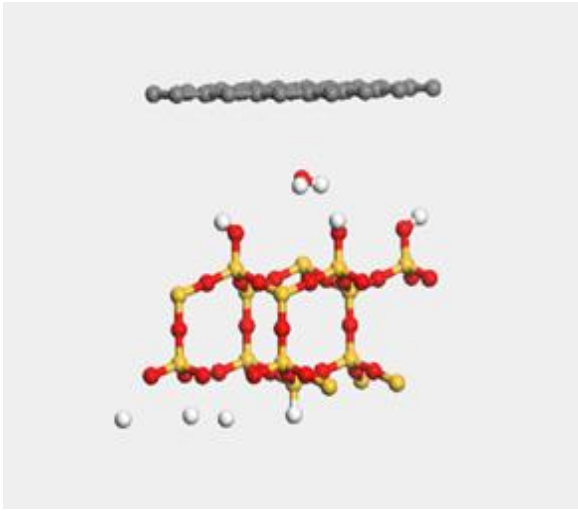
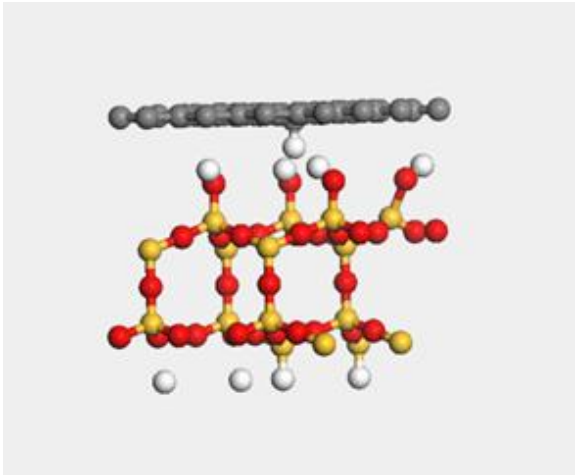


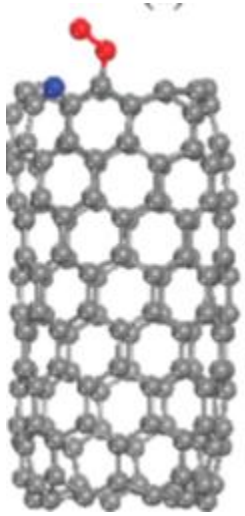
Figure 11. The simulation models we based on.



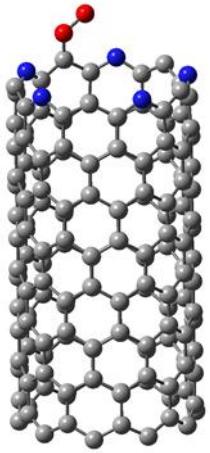


Simulation on N-CNTs system

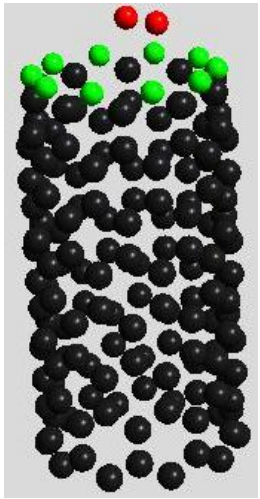
In this work, we studied the Carbon nanotubes (CNT) based structure as catalyst which is used for the oxygen reduction reaction (ORR) in the fuel cell cathodes.



(a)



(b)



(c)

Tools

- VASP package

VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set.

- Materials Design
- MedeA

MedeA® is designed for materials engineers and scientists who want rapid and reliable answers for a range of materials issues related to application areas such as electrical power generation, automotive applications, energy storage, alloy design, microelectronics, the chemical industry and petrochemicals.

Tools

- DL_POLY

DL_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith

- LONI machines

Acknowledgement

These works are supported in part by the NSF-LASiGMA program (grant number #EPS-1003897), the LaSPACE/NASA (grant number NNG05GH22H), DOE award No. DE-FE0004734 and DE-FE0003693, and the LONI institute.

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Thank you

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