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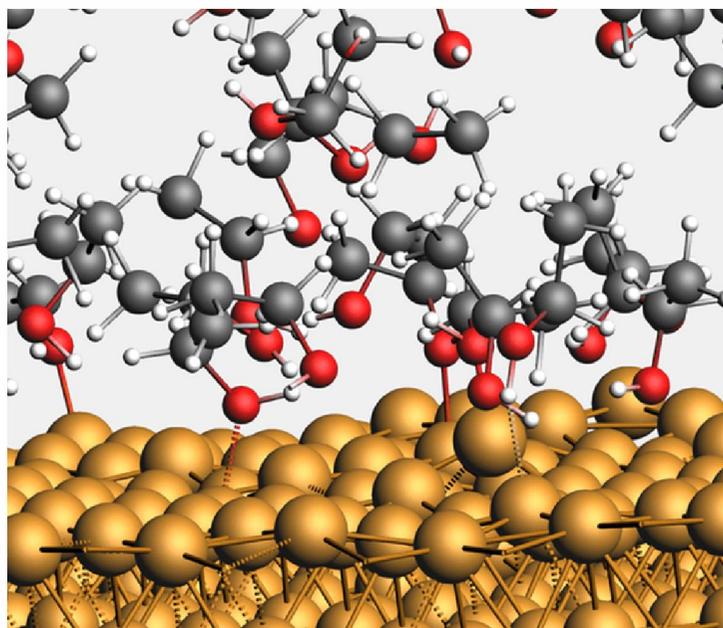
THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES

Multis

27-30 June 2022, Krakow, Poland



The effect of solvent on oxidation behavior of copper during laser irradiation of suspension, a reactive bond molecular dynamics study



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Laboratory of laser-matter interaction

Making sub-micron composite powders using Pulsed Laser Irradiation in Liquid (PLIL) method

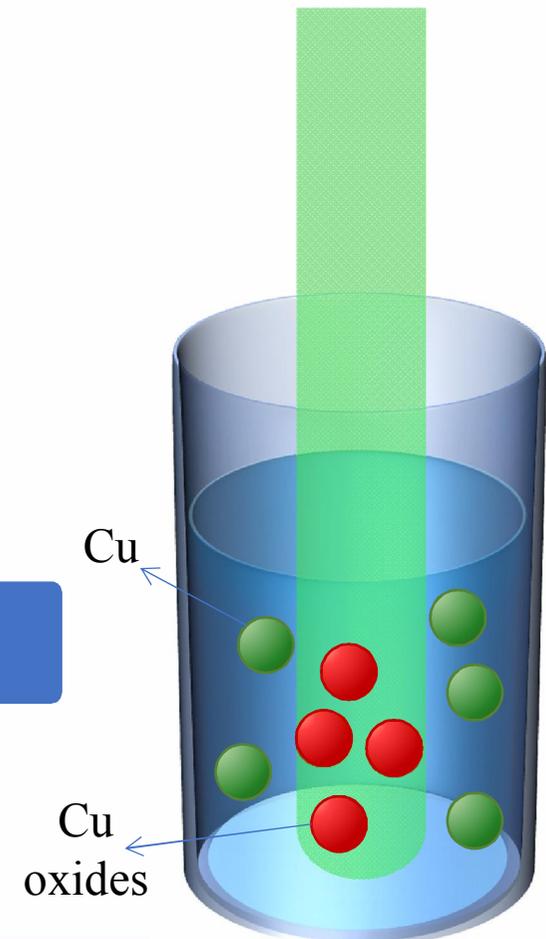
Irradiation process & characterization of final powder

Thermodynamical calculations of stability diagrams

Temperature calculation of spheres and solvents

Molecular dynamics (MD) study

Density functional theory (DFT) study



Why Cu oxidation is important?

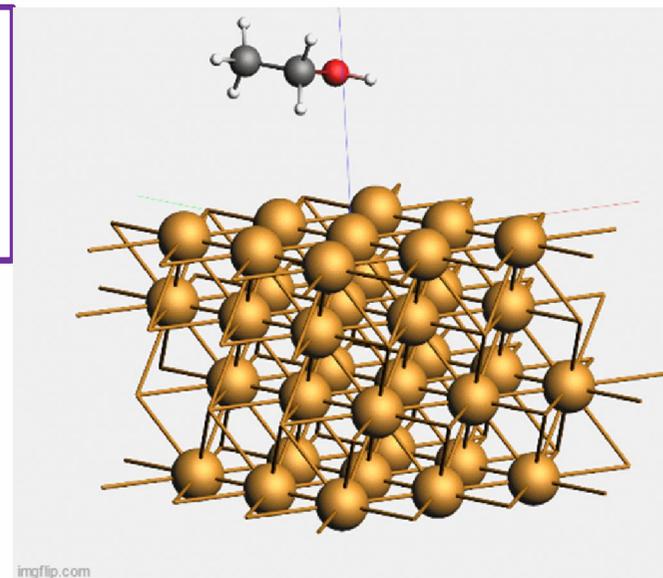
- Give us the knowledge of making heterojunctions
- Applicable in bio-materials and green energy production



Modeling details

- Software: AMS
- Module: ReaxFF
- Method: Reactive bond force field
- Ensemble: Canonical (NVT)
- Boundary: Periodic in all directions
- Slab: Cu (111) plane
- Force Field: Zhu, Wenbo, et al. "Development of a reactive force field for simulations on the catalytic conversion of C/H/O molecules on Cu-metal and Cu-oxide surfaces and application to Cu/CuO-based chemical looping." *The Journal of Physical Chemistry C* 124.23 (2020): 12512-12520.

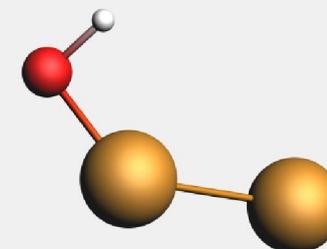
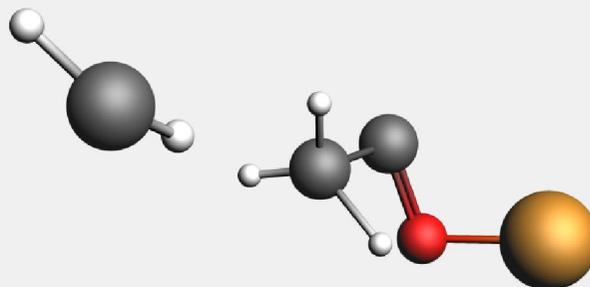
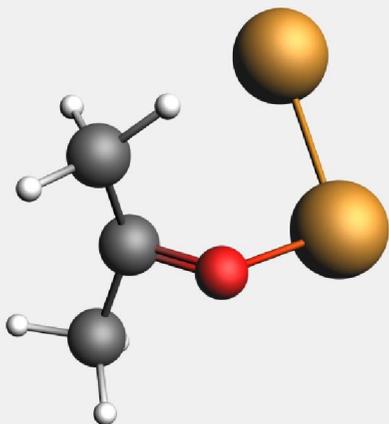
Yellow : Copper
Red: Oxygen
Gray: Carbon
White: Hydrogen





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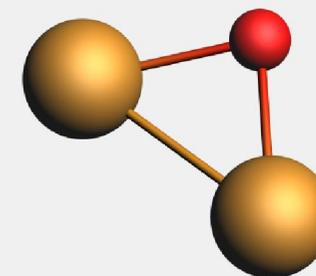
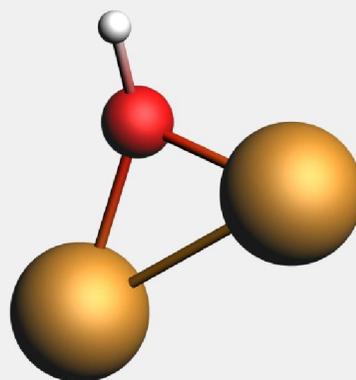
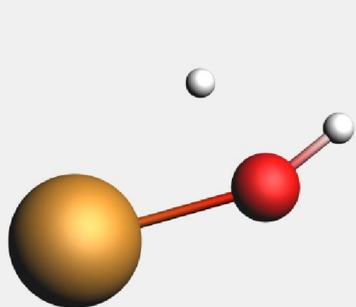
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time/ps 3.6

4.8

10.5



10.9

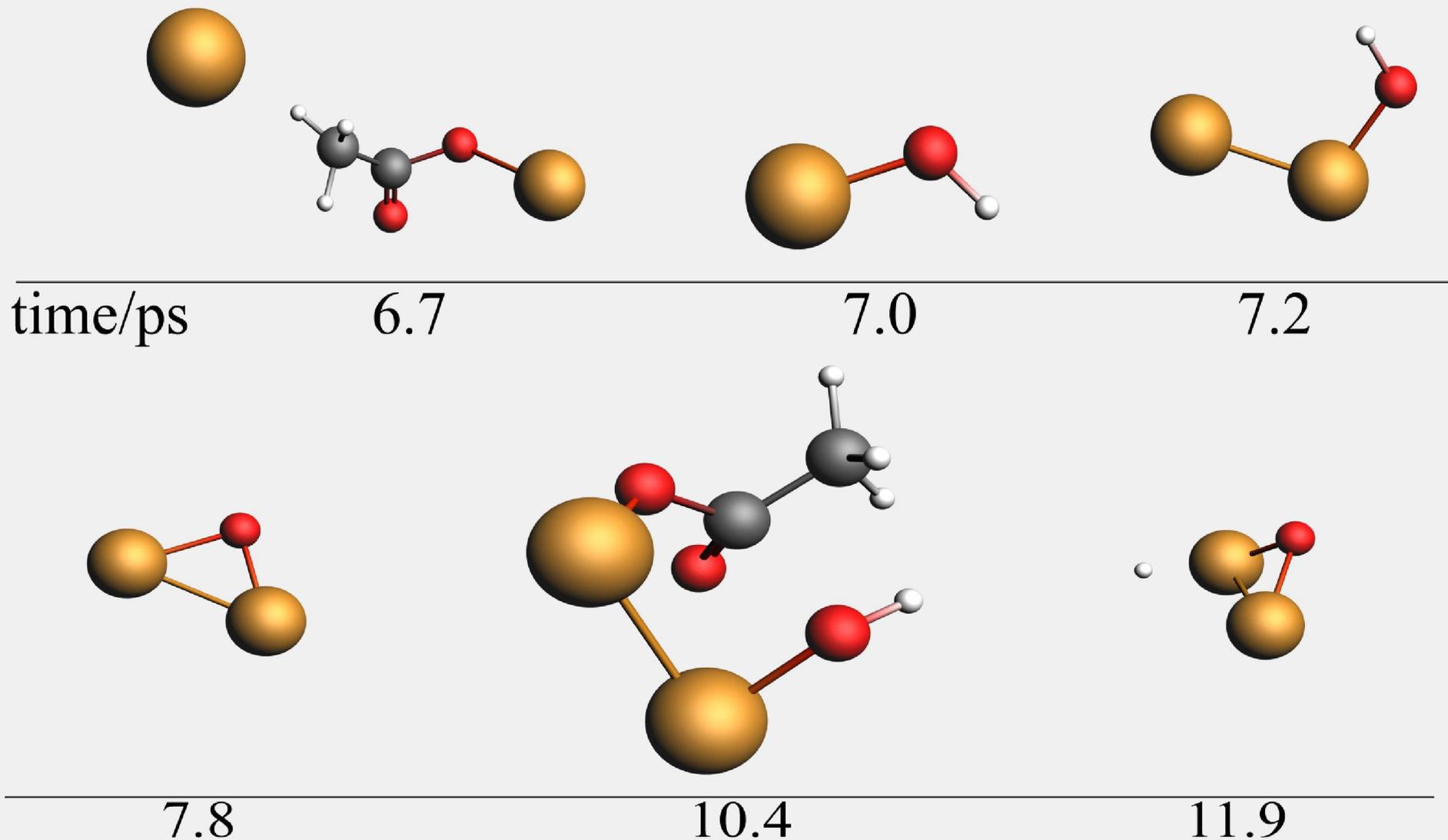
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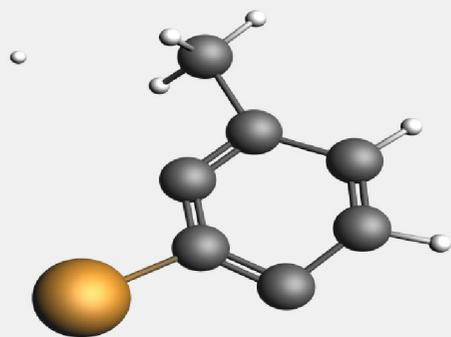
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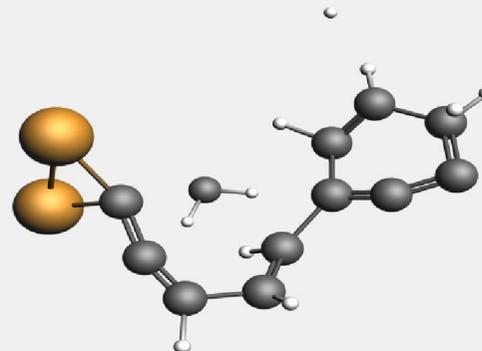
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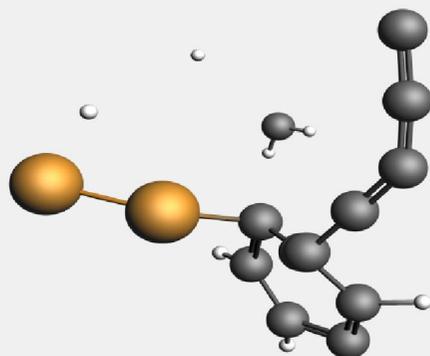
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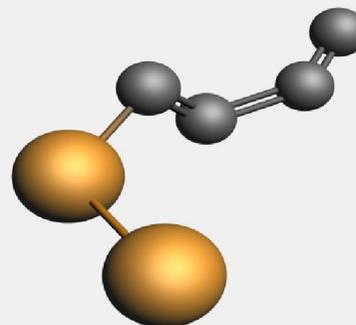
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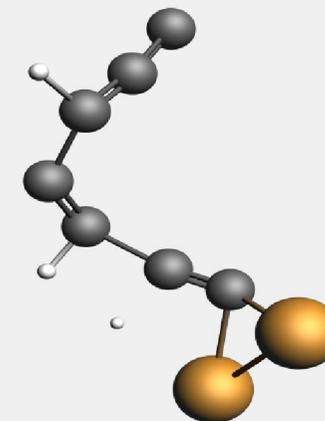
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21.1



23.4



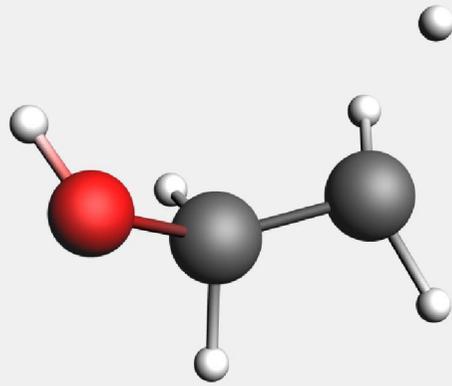
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time/ps

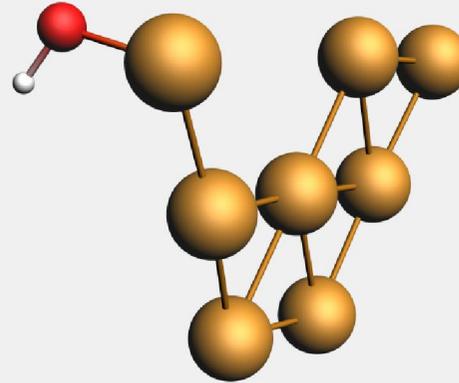


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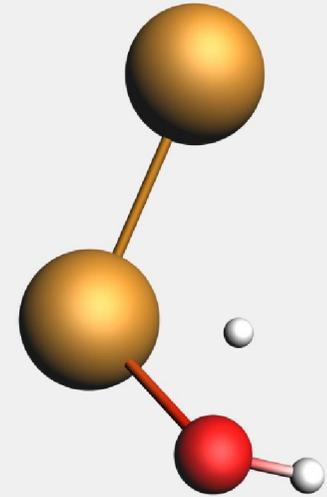
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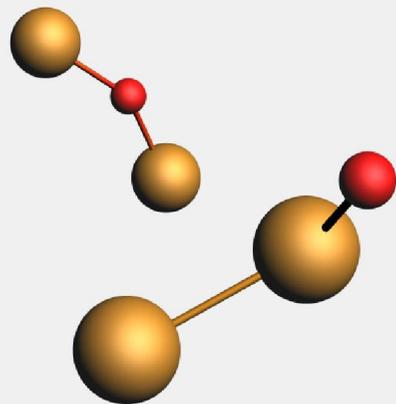


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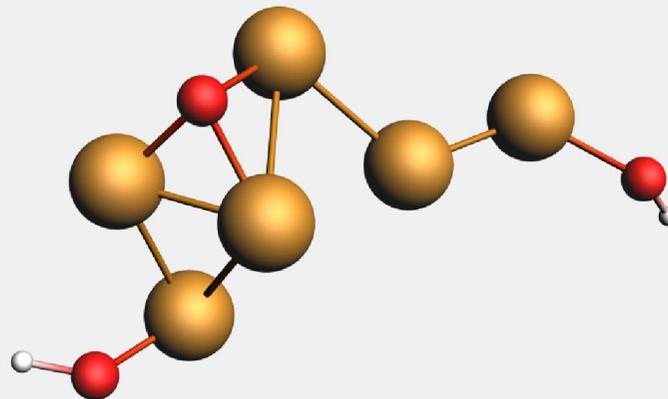


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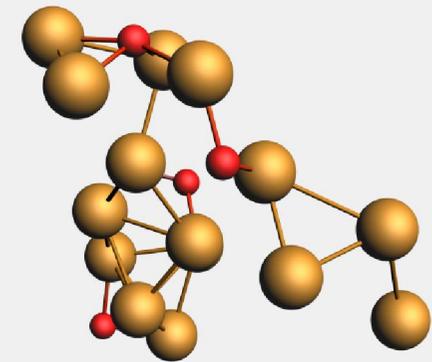
time/ps



9.5



10.9



72.7



Conclusions

- Oxygen content of solvent affects the oxidation during PLIL process
- The mechanism of oxidation in ethanol, acetone and ethyl acetate is similar due to their oxidative nature including
 1. OH absorption
 2. Decomposition of solvent
 3. Surface oxidation
 4. Internal oxidation
- Toluene possesses more reduction nature

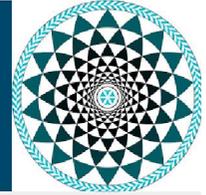




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Thanks for your attention

