Modeling LENR Chemical Environments by Computational Chemistry

Joseph Peter Guokas
joe.guokas@yahoo.com

Goal: Model the LENR Environment

Model conditions related to LENR anomalies using standard ab initio computational chemistry software, so verification is transparent and replicable. Models of the LENR environment should suggest ways it can be triggered, optimized, and tested.

I have been doing this modeling for years, but recently saw reports of an issue that could throw doubt on the validity of these models.

Issue: Point Nucleus Artifacts

It has been reported that models representing the nucleus as a point charge may create artifacts that appear as small, deep exotic orbitals.

The reports say the suspect orbitals do not appear when the nucleus is modeled as a charge distributed over a finitely small region. [1][2]

Conclusion: We should use software that allows us to select point nucleus model or finitely small nucleus model, to see if the change impacts our results.

Preventing other artifacts

There are other conceivable sources of artifacts that should be vetted by varying these factors :

- Computational methods
- Basis sets
- Grid spacings
- Assumed multiplicities (especially exotic orbitals)
- Corrections for relativistic orbitals (especially exotic orbitals)

Suggested software for standard

Standard software for our community could help in several ways:

- Testing each other's results
- Building on each other's results
- Collaborating
- Warning others of quirks of packages in the unusual environment of exotic chemistry
- Cheaply, easily testing by outsiders at national labs and CERN

Suggest these packages, based on ability to handle exotic chemistry and other peculiarities of LENR, cost, and usage at national labs and CERN :

- NWchem - computational chemistry package
- LAMMPS - molecular dynamics package, surfaces, defects, charged particles passing through material
- Python - scripting, for NWChem and LAMMPS
- ECCE, or Avogadro, or GaussView - for viewing, building
- Scientific Linux - OS used by national labs and CERN, stressing version stability for ease of collaboration

This list is based on my limited experience, so suggested alternatives are welcome.

What was learned

- Computational chemistry software showed interesting properties of the LENR environment, but methods must be verified.
- Point nucleus models are suspected to create artifacts that appear as exotic orbitals.
- We should use software that can compare results of point nucleus with finitely small nucleus.
- To ensure against other artifacts mentioned above, vary the suspect factors.
- If exploring exotic orbitals, be aware that software packages can have limits on how small an internuclear distance is permitted, or can have problems converging to a valid result if that distance is too small.
- If exploring exotic orbitals, software packages that provide accurate NMR results may be best for modeling the environment near the nucleus.

Next Steps

- Rerun my existing simulations with other software to verify them with finitely small nuclei.
- Continue learning properties of LENR environment through computational chemistry.
- Welcome any suggestions of good software to consider as standard for our community.
- Welcome any suggested alternative ideas for LENR environments, to examine with computational chemistry.

[1] A. Rathke, *New J. Phys.* **7** (2005) 127.

[2] B. Ritchie, *J.Condensed Matter Nucl. Sci.*, **11** (2013) 101-122.