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Electron Screened and Enhanced Nuclear Reactions

ICCF-24 Solid State Energy Summit

July 25-28, 2022

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V1.1

Outline

1. Electron Screening, U_e
   - Astrophysics
   - Laboratory Astophysics
   - Terrestrial
   - LENR and LCF
2. Enhanced Screening: ^{7}Be Model System
3. Density Functional Theory Modeling
4. Conclusion
5. Acknowledgements

Electron Screening

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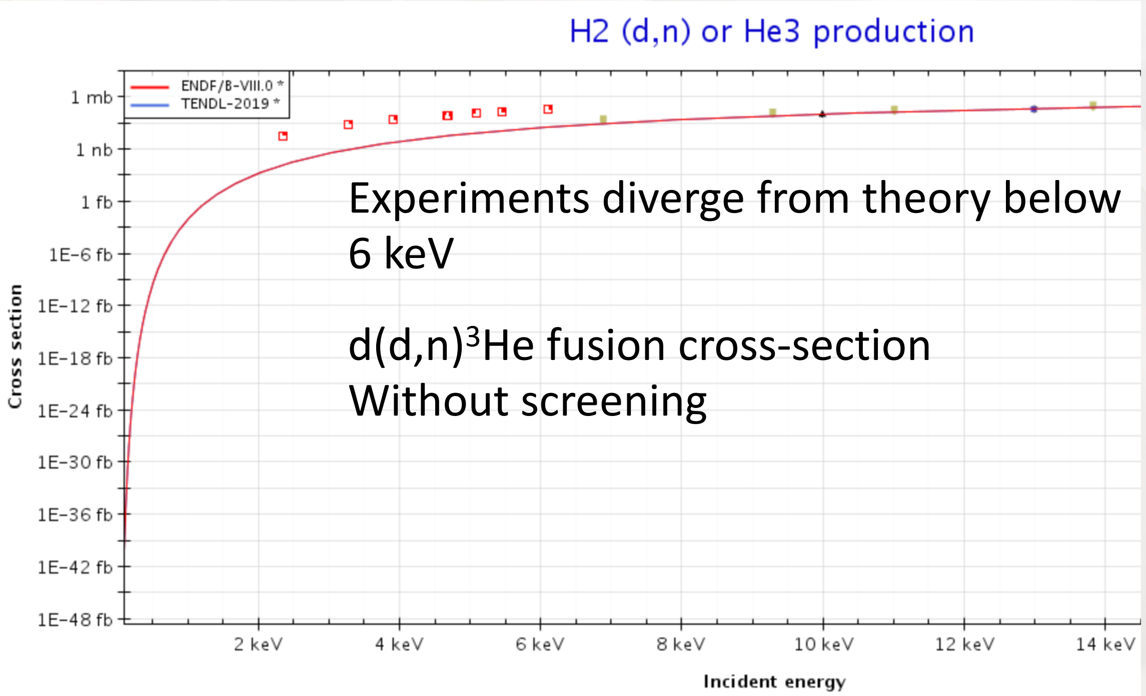
1. **Astrophysics**
    1. Strong and Weak screening:
       Salpeter, 1954
    2. Fermi Degeneracy, ≈ 10^{23} e^{-}/cm^3
    3. Holds up white dwarf stars
2. **Laboratory Astrophysics**
    1. Accelerator studies
       Rolf, Czerski, Huke et al., 1980s
       Bystrisky, Kitamura, 2000s
    2. Gamow Factor Enhancement
       Pines, 2020
3. **Terrestrial**
    1. Metal Conduction bands, ICF
4. **LENR and LCF**
   Srinivasen, 1991
   Schenkel, 2019

$^7Be_4$ has astrophysical significance

Radioactive but whose EC decay rate can be modified by compression. *(^{8}Be is unstable and decays to 2 α!)*

The center of the Sun has a density of 150 gm/cm^3 and a pressure of 26.5 million Gpa

This will affect the decay rate of ^{7}Be at the solar core and the ^{8}B neutrino flux.



https://www.oecd-nea.org/janisweb/book/deuterons/H2/MT4/renderer/220

Pd Lattice Screening Potential Calculation[1]

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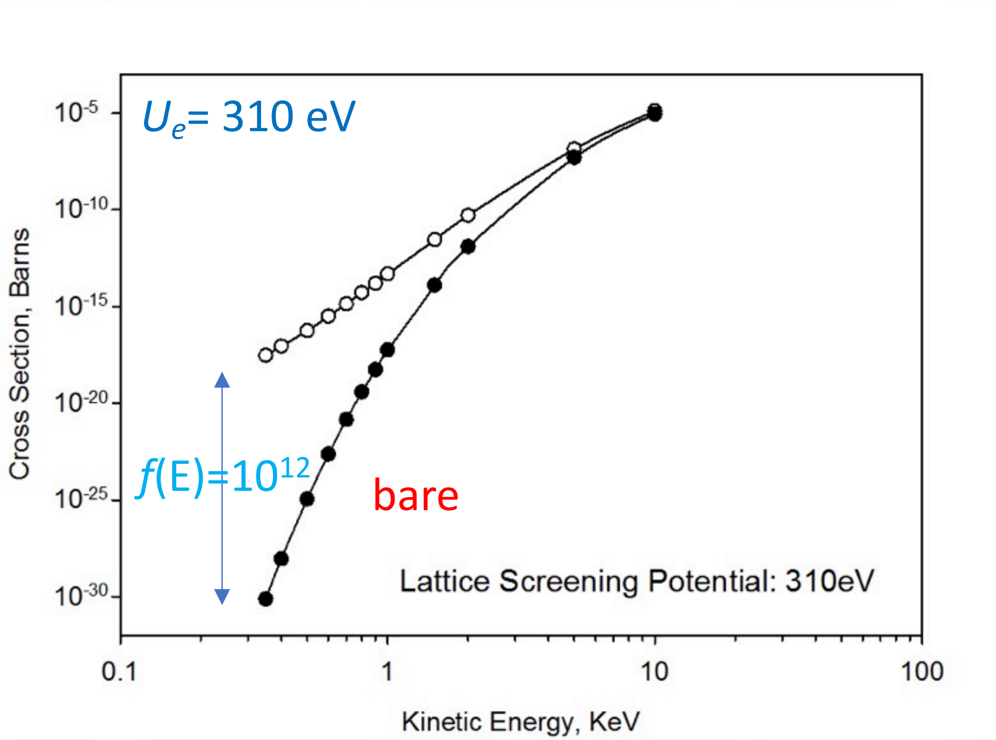
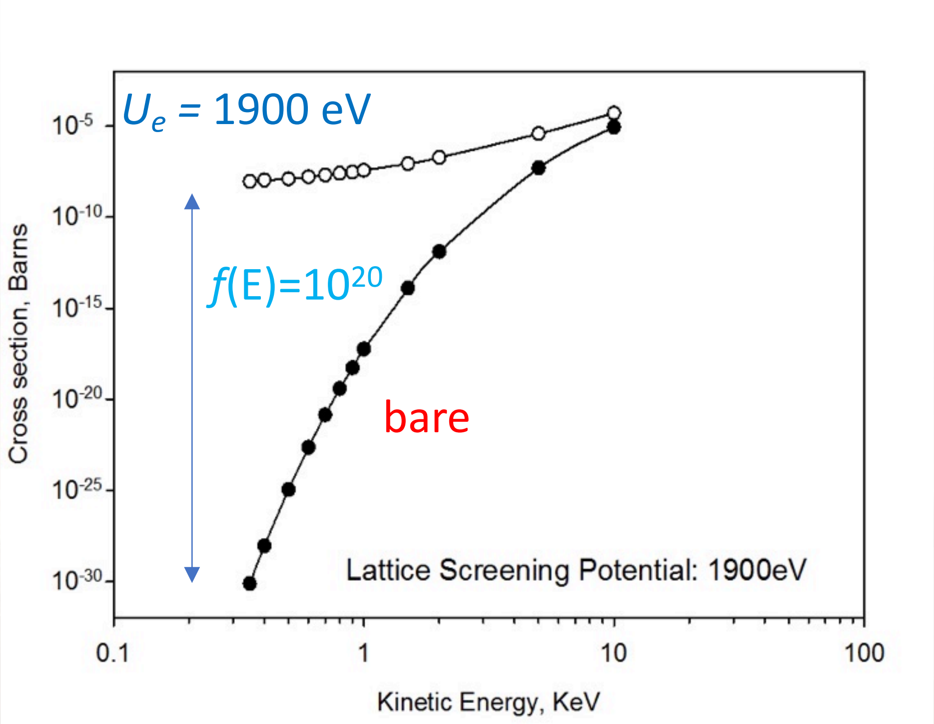




K

Bare cross-section $$\sigma_{bare}(E) = S(E) \cdot E^{-1} \cdot \exp(-G(E))$$

Enhancement factor $$f(E) = \frac{E}{(E+U_e)} \cdot \exp\{G(E) - G(E+U_e)\}$$

Enhanced Experimental cross-section $$\sigma_{exp}(E) = \sigma_{bare}(E) \cdot f(E)$$

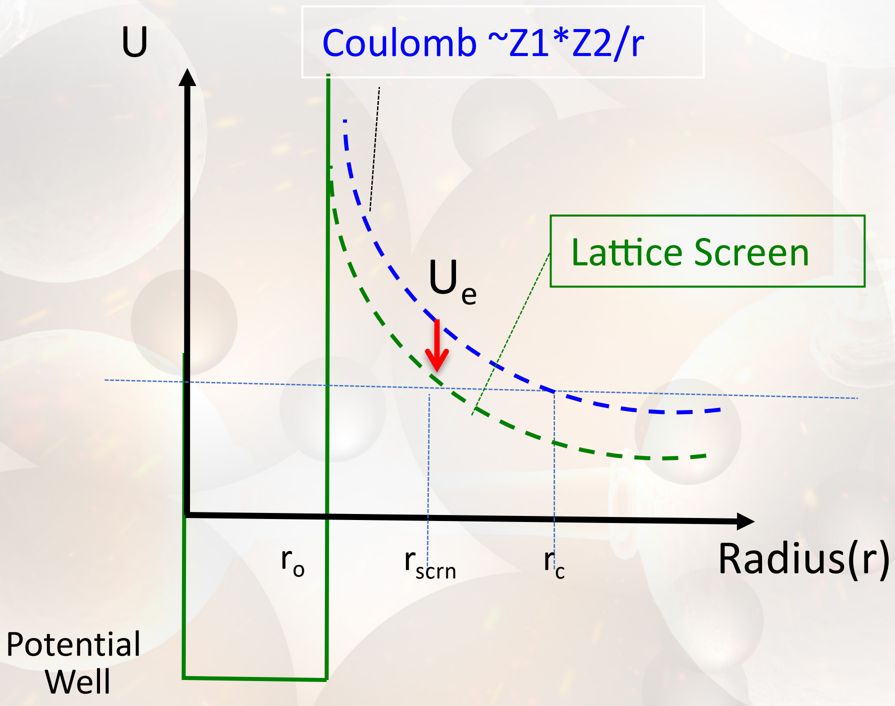
E Kinetic Energy, keV
U_e Electron Screening, keV
G(E) Gamow Factor
S(E) Astrophysical Factor

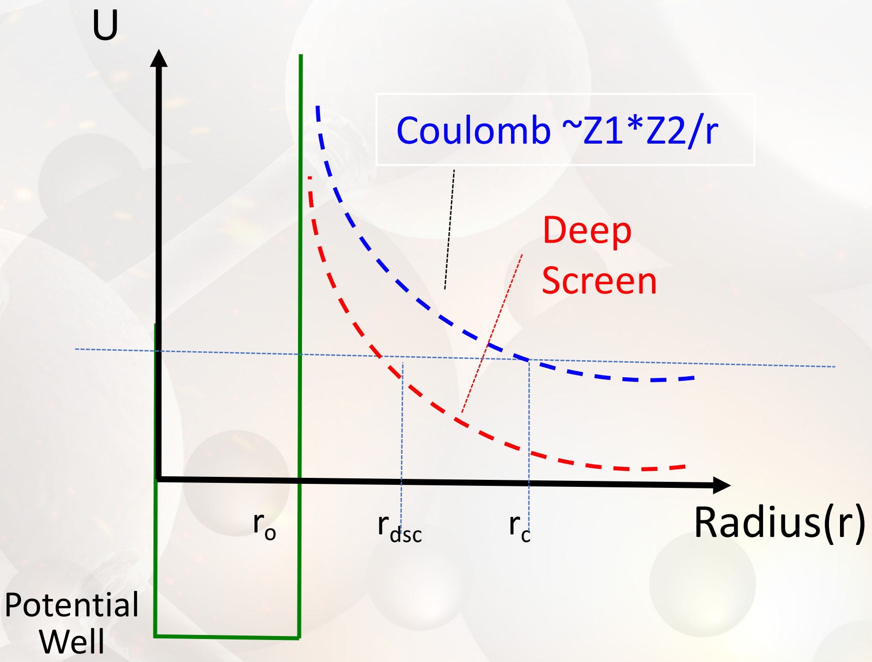
Screening works below 10 keV Kinetic Energy and increases nuclear reaction rates by potentially 20 orders of magnitude.

[1] Calculations by V. Pines and M. Pines, NASA Advanced Energy Conversion Project

Comparison of Lattice vs. Deep Screening[1.]

How to increase deep screening?





Glow Discharge or Plasma Ion source
X-ray and gamma photon source

[1.] Calculations by V. Pines and M. Pines, NASA Advanced Energy Conversion Project

Gain: Enhanced Cross-section vs Thermal Power[1]

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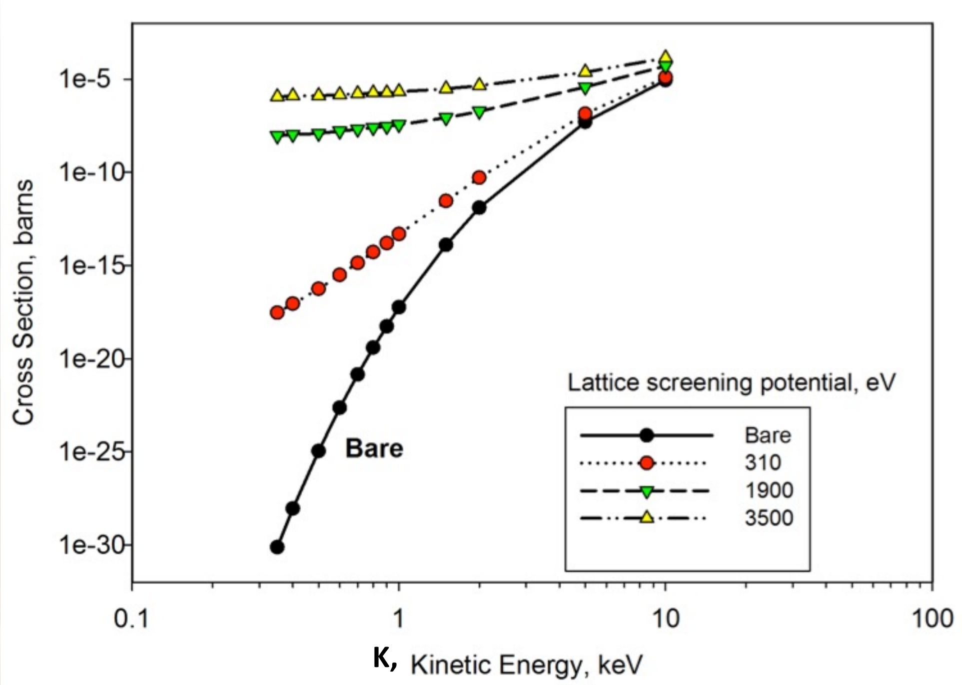
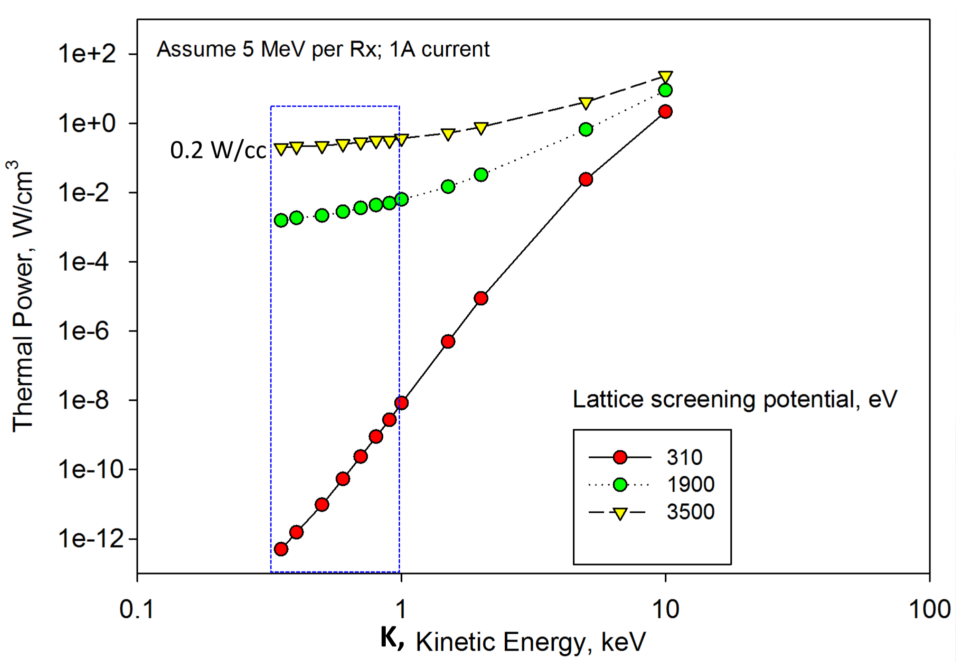
Cross Section vs Kinetic Energy



Specific Thermal Power vs Kinetic Energy



- Lattice screening:
  - Key parameter for reaction scale-up
  - More effective at lower energies
- Material composition/microstructure can be combined with other physical parameters (fields, plasma current, pulse, other) to increase thermal power output
- Specific power calculation assumed only primary D-D fusion reactions (~5 MeV/Rx)
  - Subsequent cascading reactions expect 4-5x increase→1000 W_{th} (1000 cc material)

[1] Calculations by V. Pines and M. Pines, NASA Advanced Energy Conversion Project

Enhanced Screening: ^{7}Be Model System

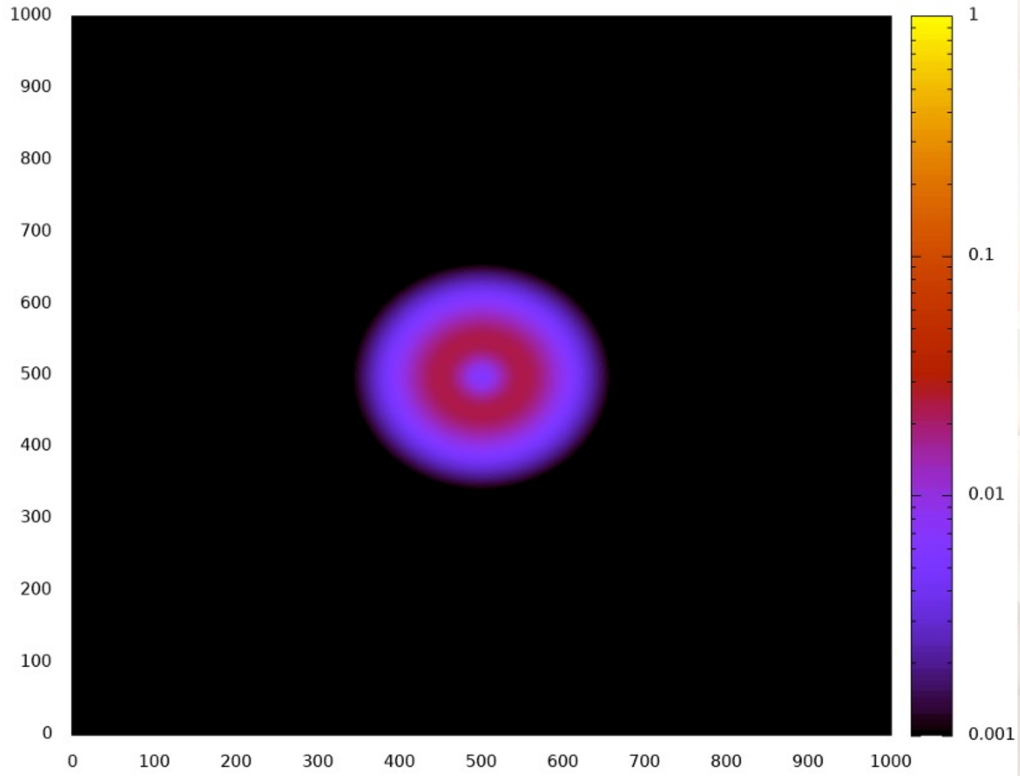
- ^{7}Be has astrophysical significance:
  - The decay rate in stellar cores effects the ^{8}B neutrino flux.
- It can be prepared terrestrially to study changes in half-life using the reaction:
  - $^{7}Li(p,n)^{7}Be$, then
    - ^{7}Be decays by electron capture (EC) to ^{7}Li with a half-life, $t_{½}$, = 53.12 days
    - ≈ 10.4% probability ^{7}Be decays to the first ^{7}Li excited state 3/2-
    - emitting 477.6 keV γ -ray photon.
- A 0.8% change in ^{7}Be $t_{½}$ has been observed (and DFT modeled) when placed within:
  - Fullerene (Buckyball)
  - Interstitial Pd
  - Diamond Anvil
- *Demonstrates a chemical environment interacts with a nucleus*
- *Density Functional Theory can model these effects*

Ab-initio (*First Principles*) Computational Lattice Design

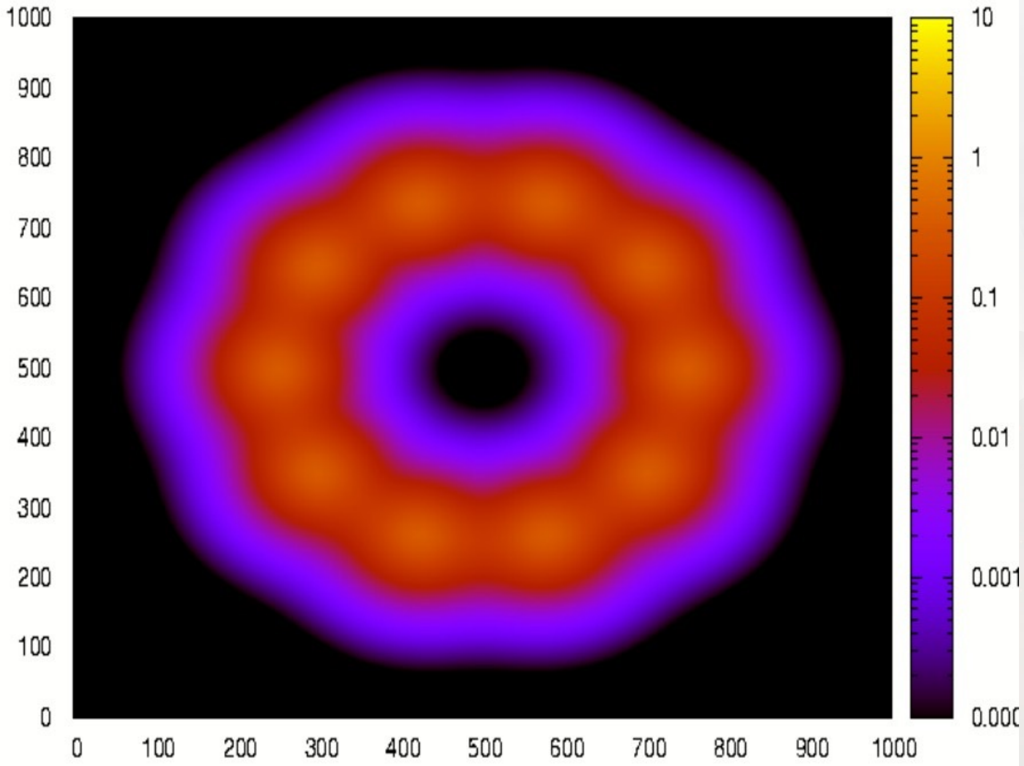
- Density Functional Theory (DFT) *e.g. Quantum Espresso, VASP, WIEN2K,etc*.
  - Solve the approximate Schrödinger equation in a solid lattice
  - Provides band structure and local electron density
  - Can calculate complex, inhomogeneous lattices and interfaces
  - Can incorporate external EM fields
- Evaluate complex hydrogen isotope-lattice interactions
- Evaluate potential suitability of alternative elements, alloys, and structured materials (superlattice)
- Limitations
  - Pseudo-potentials for *Z>4* (Beryllium, $^{A}Be_{4}$) limited to valence electrons
    - Resolved by additional pseudo-potential file calculations to include core electrons
  - Iterates to 0°K ground state, (e.g. not room-temp 273 °K or higher)
    - *Can be resolved by more computationally intensive dynamic calculations.*

DFT modelling of Be $2s^2$ and C_{60} $2p^2$ electron density

Modeled valence shells of Be and C only



Be $2s^2$



C_{60} $1s^2$ $2s^2$ $2p^2$ but only the $2p^2$ valence orbital modeled

Embedded Be, modelling $2s^2$ orbital

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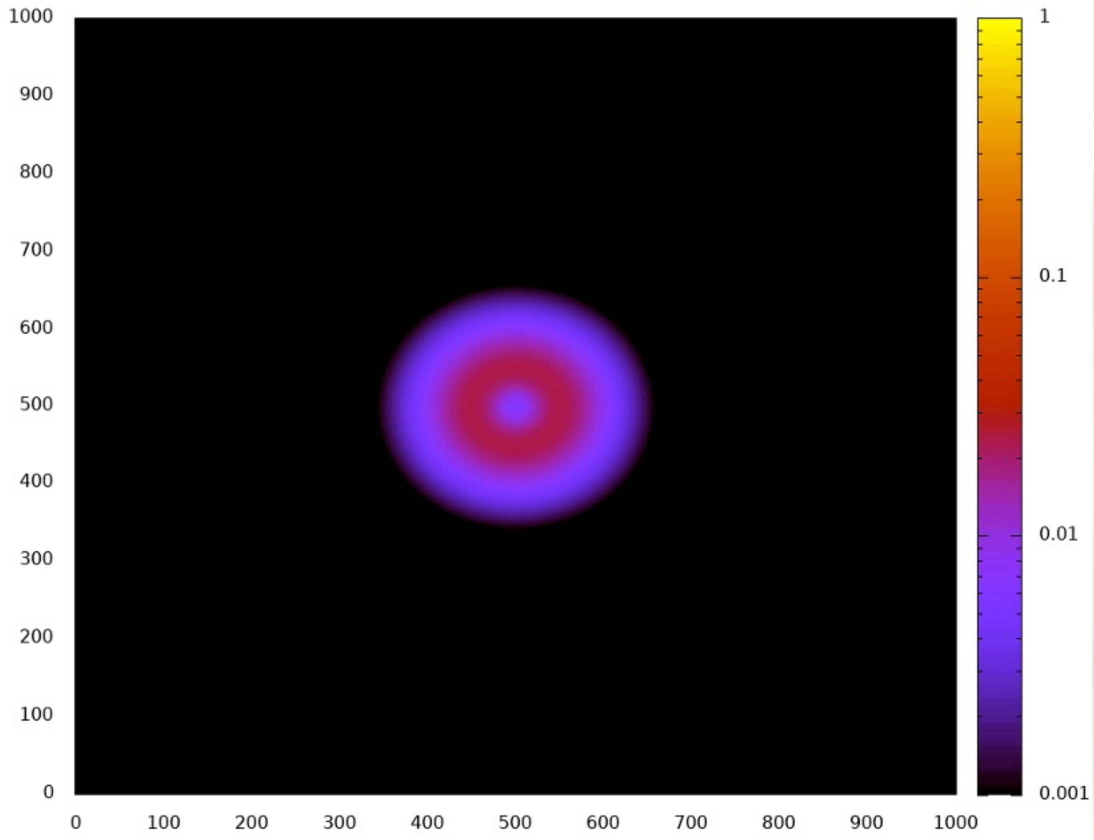
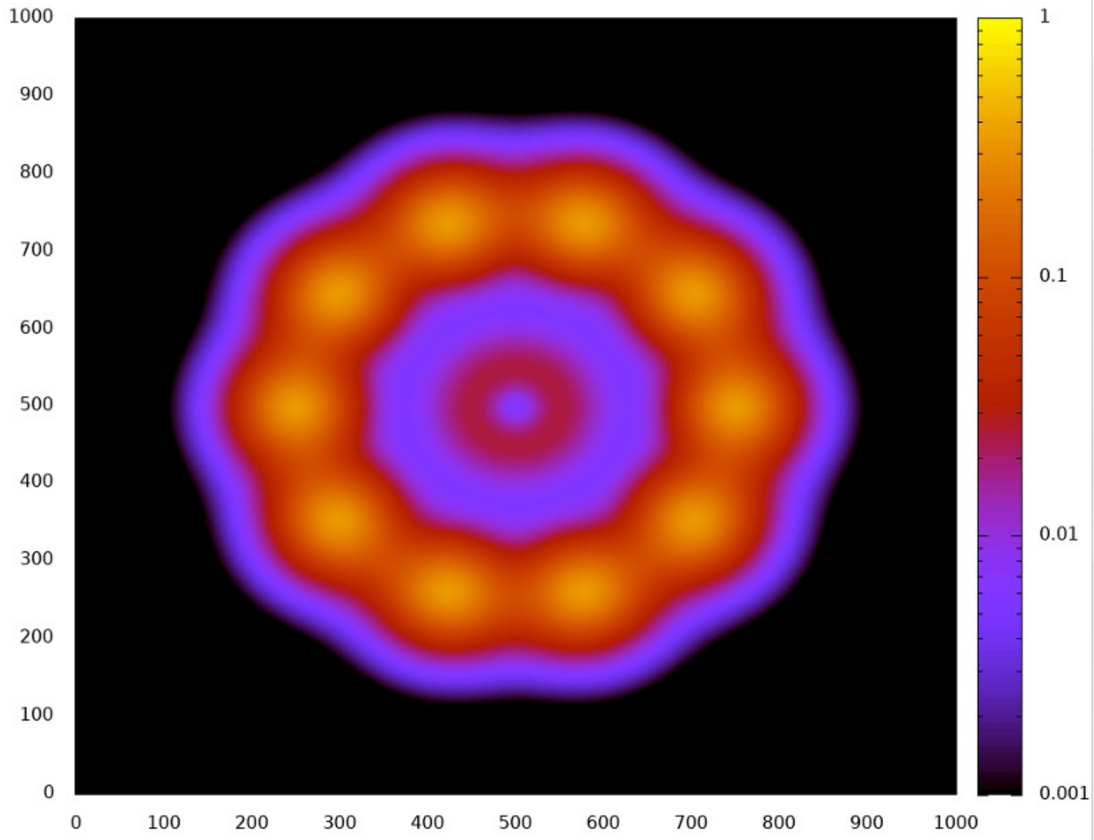
1 % decrease in electron cloud volume

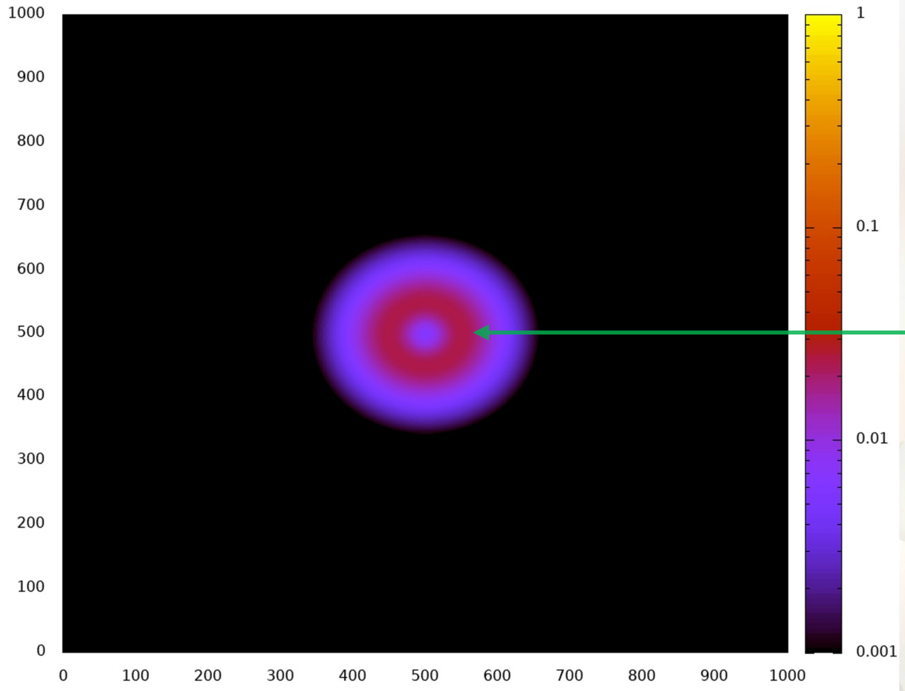


Bare Be

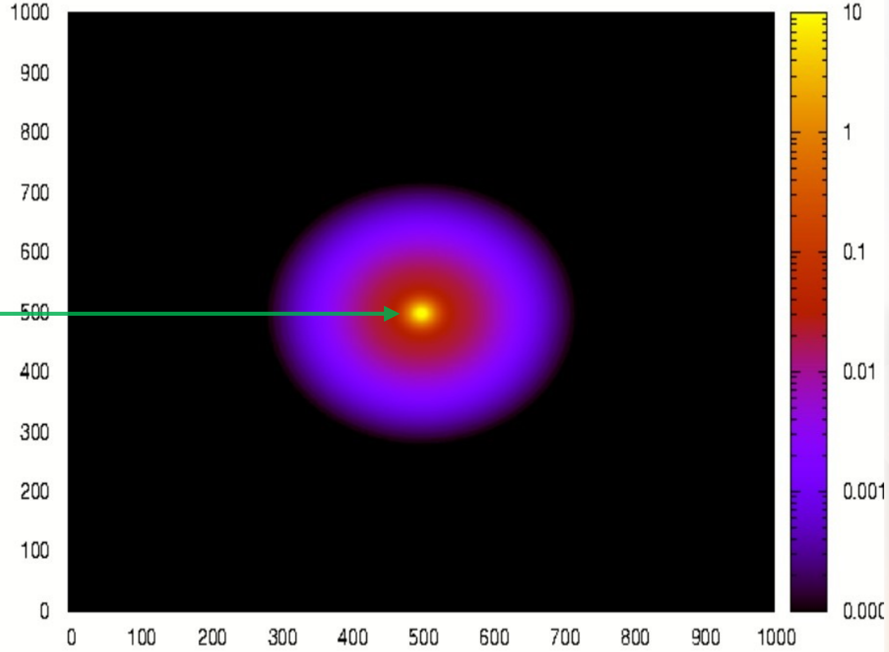


Be embedded within C_{60} Fullerene "buckyball"

Comparison of Be $2s^2$ and $1s^2 2s^2$ electron densities



Be $2s^2$ shell



Be $1s^2$ and $2s^2$ shells

Higher electron density calculated at nucleus by including both Be shells!

Be & Embedded Be, using Be $1s^2\, 2s^2$ orbitals

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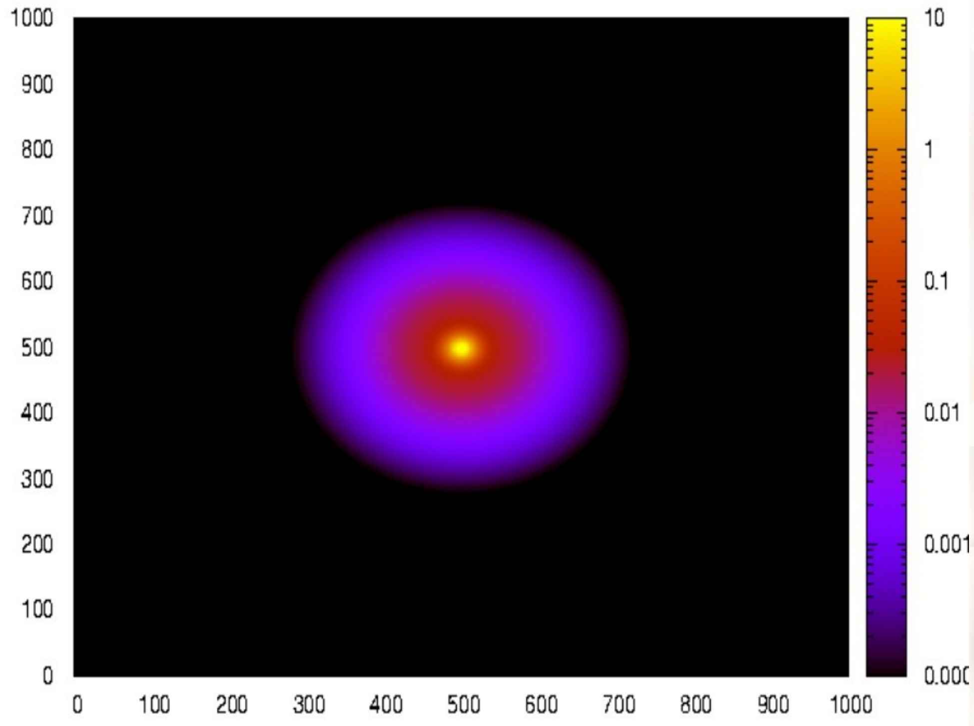
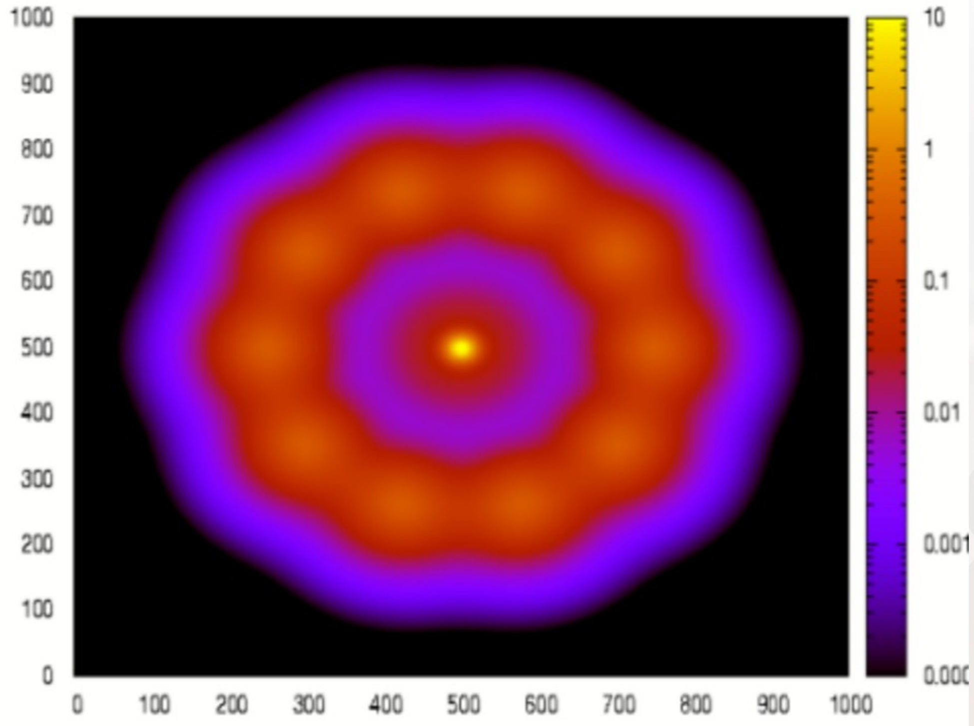
.1% decrease in electron density, but



Bare Be



Be embedded in C_{60}

Electron Density Within a Bohr radius $(5.3 \times 10^{-11} m)^3$ volume

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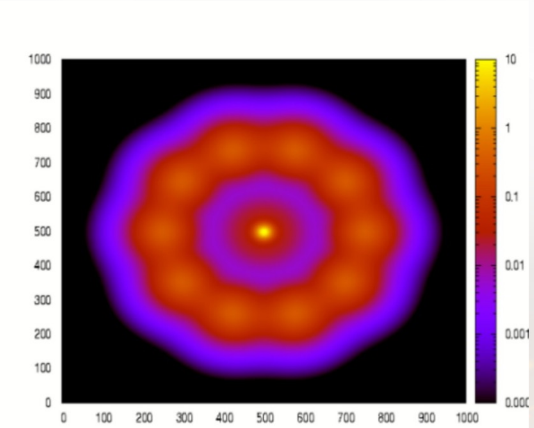
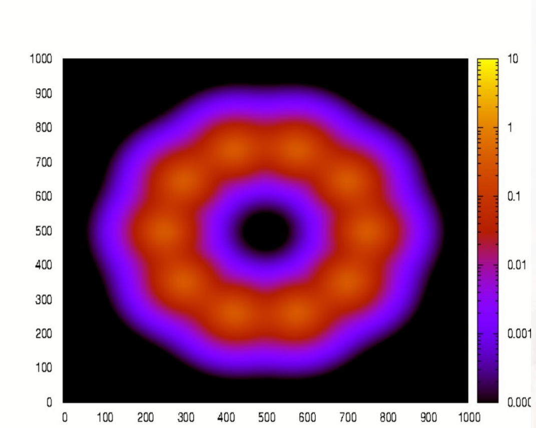
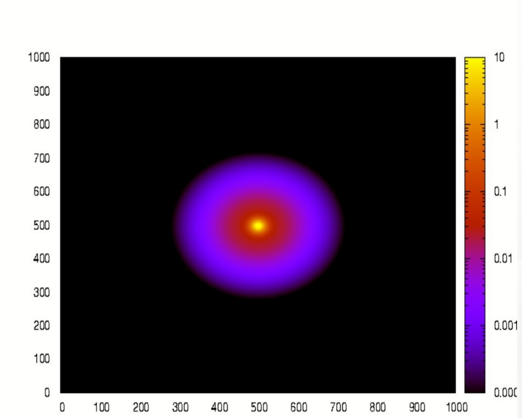

Be embedded in C_{60}

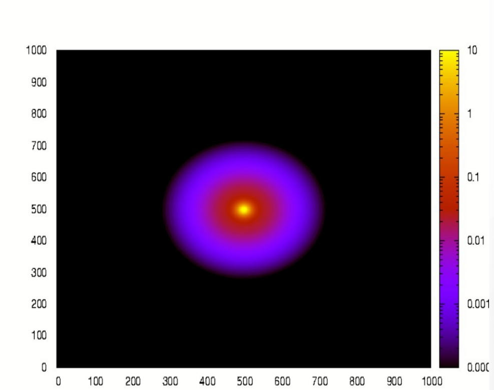
−

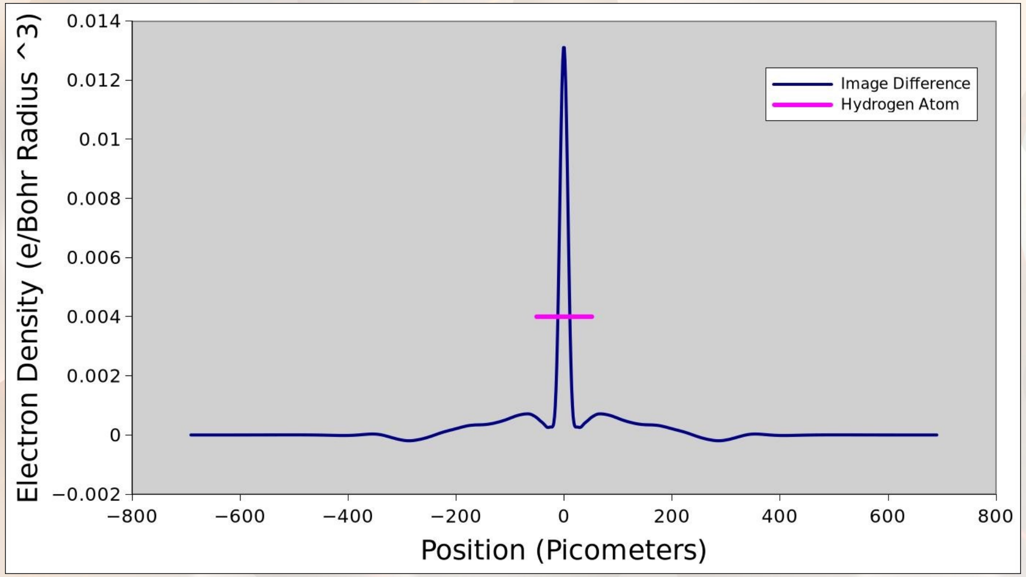

C_{60} alone

−


Be alone

=

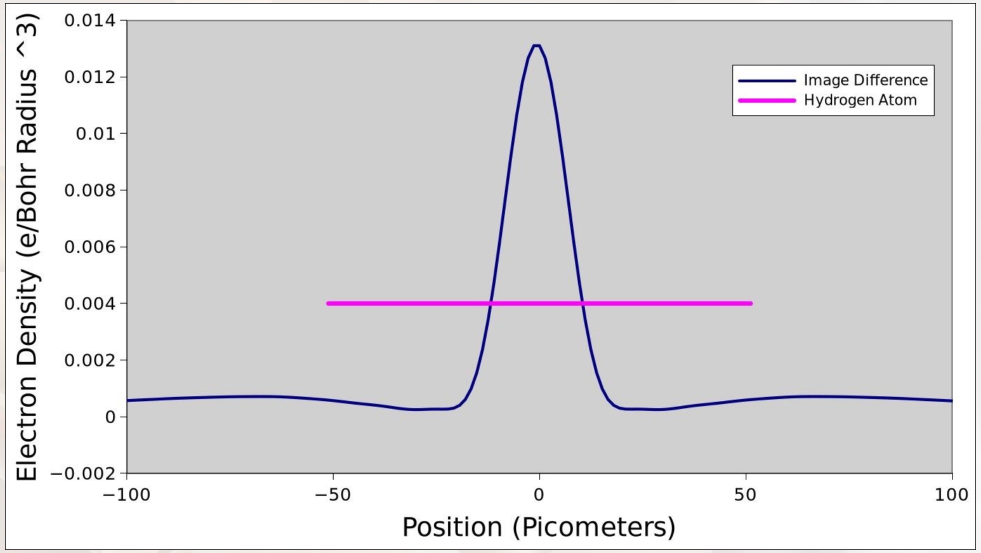

.1 % Be compression



Broad electron density after subtractions

.1% compression gives > 10x higher electron density in Be nucleus. Consistent with .8% reduction in *half life!*

Be nucleus is ≈ .003 pm (10^{-15} m)

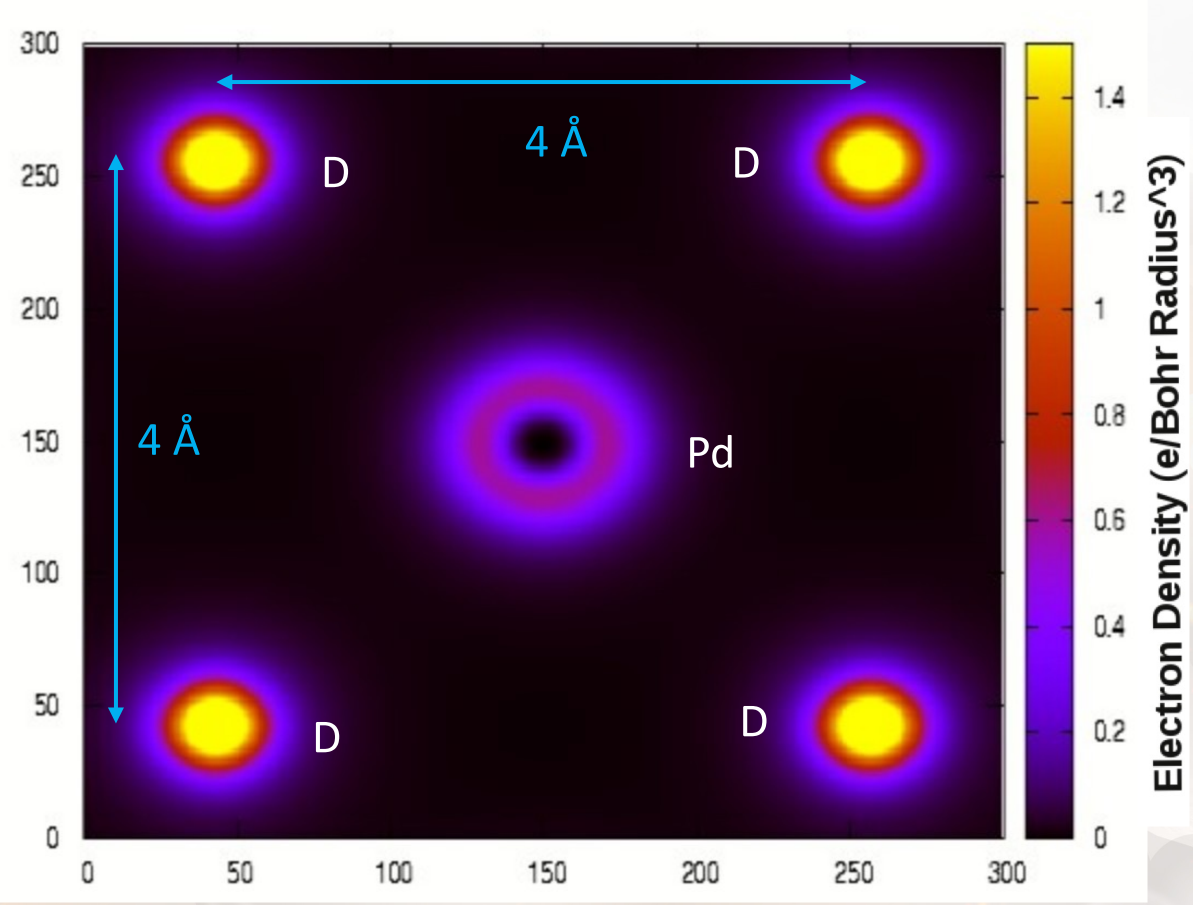


Closeup Be electron density

Pd/D and Pd CaO Lattice Electron Densities

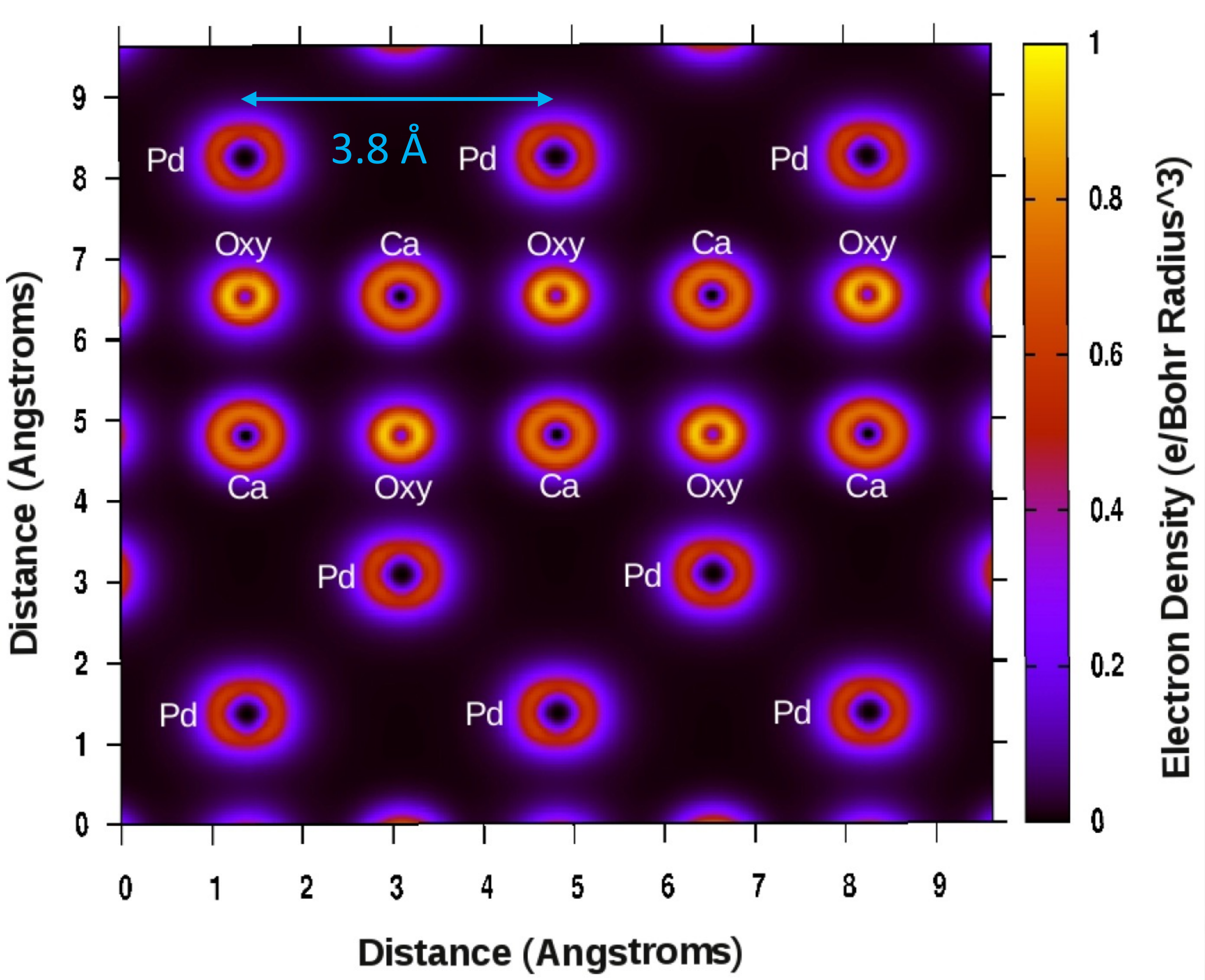
Just valence electrons

Modeling deuterium motion



Palladium Deuteride in SAV

Modeling induced ferromagnetism



Pd CaO Interface

Conclusion

- Electron screening has astrophysical and terrestrial implications
  - Stellar evolution
  - Fusion
  - Lattice Confinement Fusion
  - Low Energy Nuclear Reactions
- Occurs at high electron densities,
  - Fermi Degenerate, 10^{23} e-/cm^3
  - *Not applicable to tokamaks at 10^{14} ions/cm^3*
- Occurs at modest energies
  - *Below 10 keV*
  - *The nuclear interaction cross-section increases at ever lower energies*
- It enhances nuclear reaction rates
  - *By orders of magnitude*
- Electron screening can be modeled
  - Modeling allows optimum materials and conditions to be determined
  - Assists in guiding theory, modeling and experiment through feedback

Acknowledgements

Research conducted under:

JWK NCRADA-NSWCDD-16-191, “Low Energy Nuclear Reactions (LENR) Materials Design and Characterization”

NASA Advanced Energy Conversion Project, NNC17IA03I, “Condensed Matter Nuclear Reactions”

JWK NCRADA-NSWCIHEODTD-20-174, “Advanced Energy and Propulsion Research and Development”

NASA Lattice Confinement Fusion Project, NNC22OB04A, “NAVY-NSWC AEC Project”

With support from JWK and NASA.

With additional calculations by Dr. Vlad Pines and Dr. Marianna Pines, Senior Theoretical Physicists, NASA Lattice Confinement Fusion Project and the Advanced Energy Conversion Project.

In memorium of Dr. Marianna Pines