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Electron Screened and Enhanced Nuclear Reactions

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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

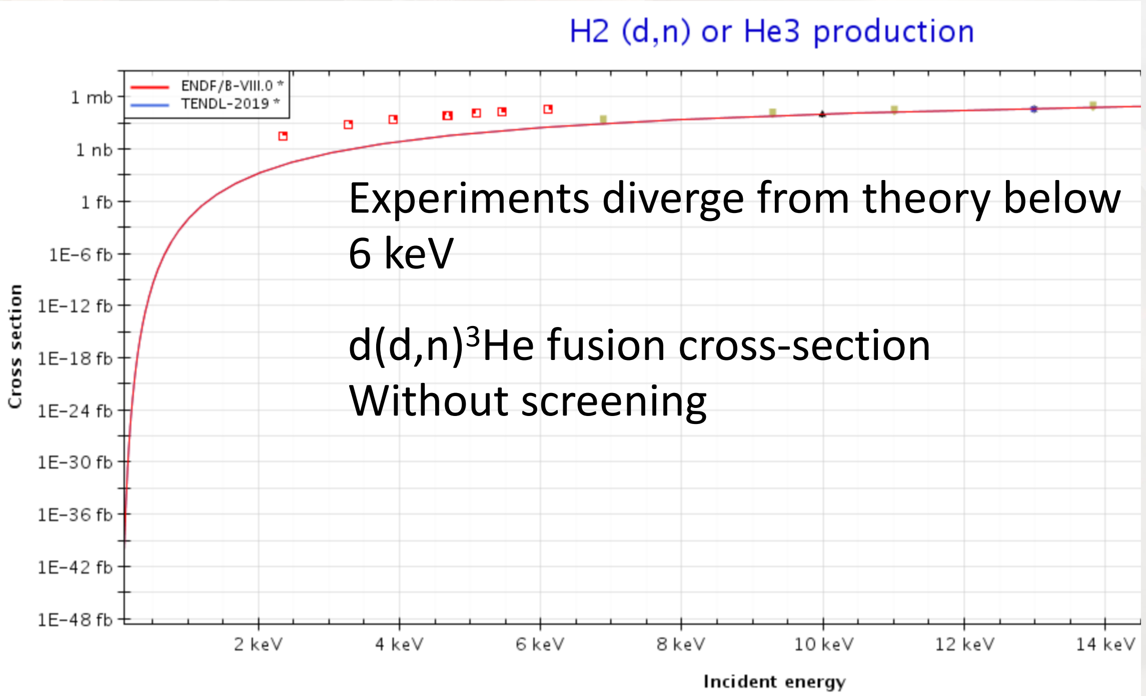
1. **Astrophysics**
   1. Strong and Weak screening:
      Salpeter, 1954
   2. Fermi Degeneracy, ≈ 10^{23} e^-/cm^3
   3. Holds up white dwarf stars
2. **Laboratory Astrophysics**
   1. Accelerator studies
      Rolf, Czerski, Huke et al., 1980s
      Bystrisky, Kitamura, 2000s
   2. Gamow Factor Enhancement
      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!)*

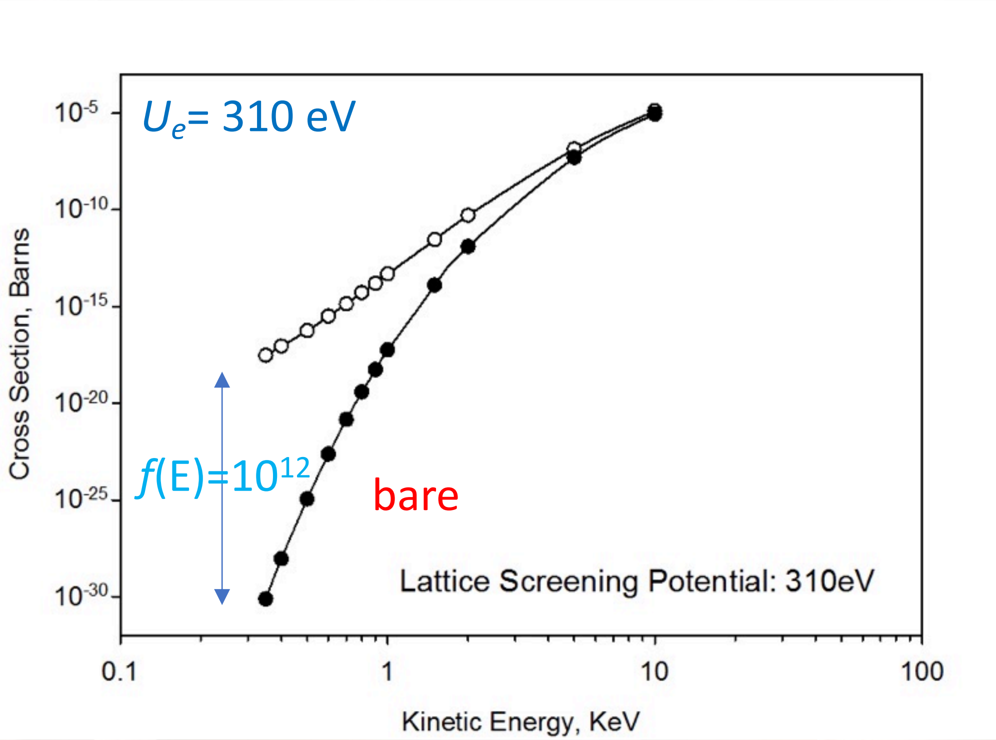
The center of the Sun has a density of 150 gm/cm^3 and a pressure of 26.5 million Gpa

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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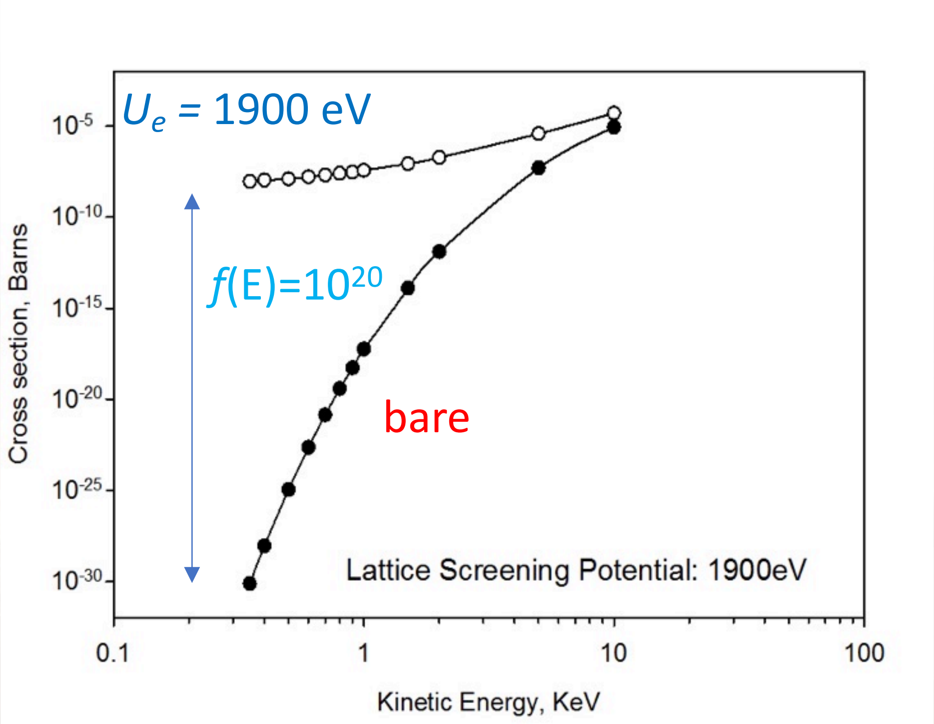


Bare cross-section $$\sigma_{bare}(E) = S(E)\cdot E^{-1}\cdot \exp(-G(E))$$

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

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

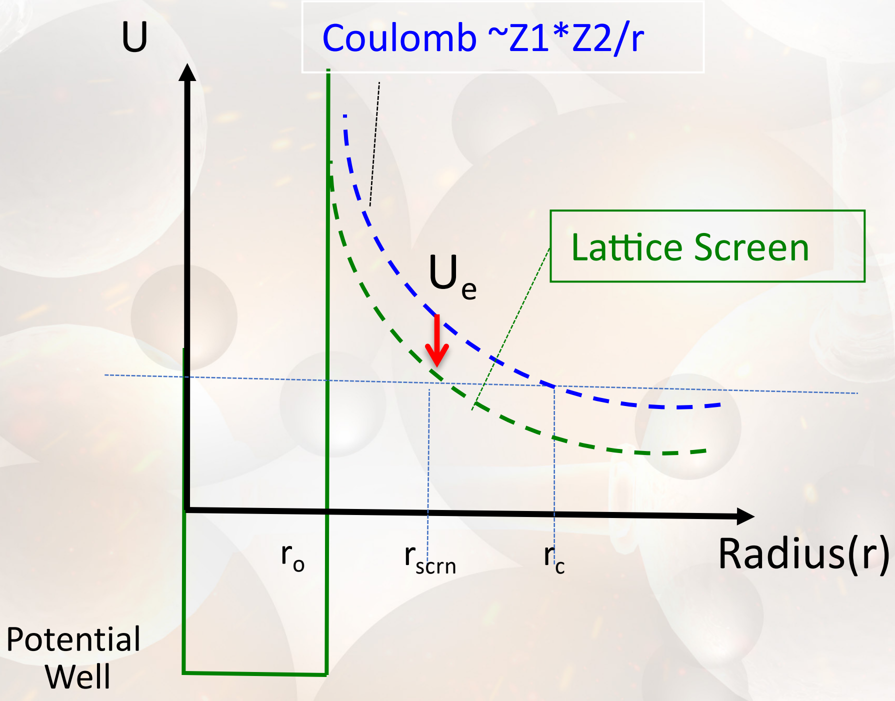
E Kinetic Energy, keV
U_e Electron Screening, keV
G(E) Gamow Factor
S(E) Astrophysical Factor

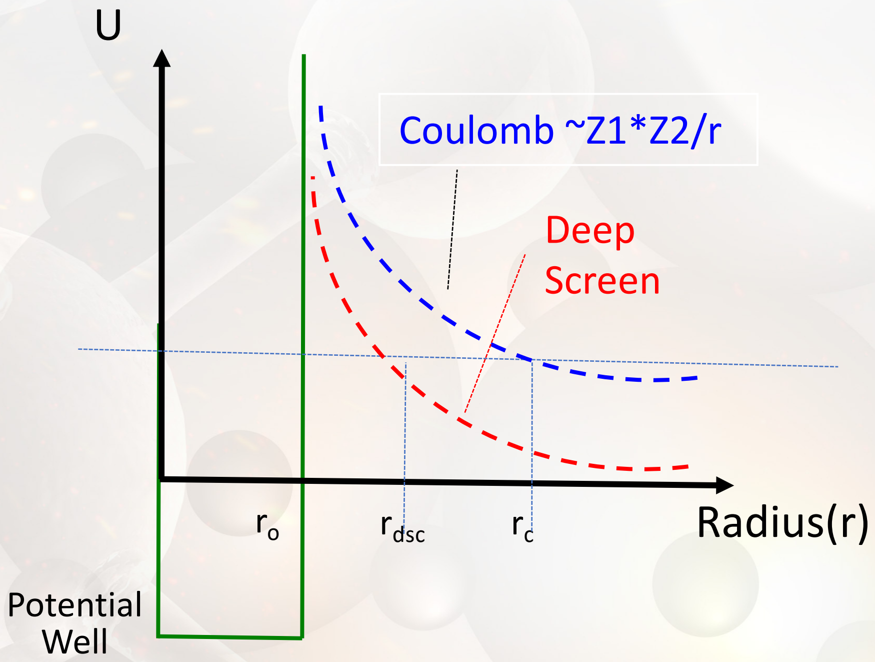
Screening works below 10 keV Kinetic Energy and increases nuclear reaction rates by potentially 20 orders of magnitude.

[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?



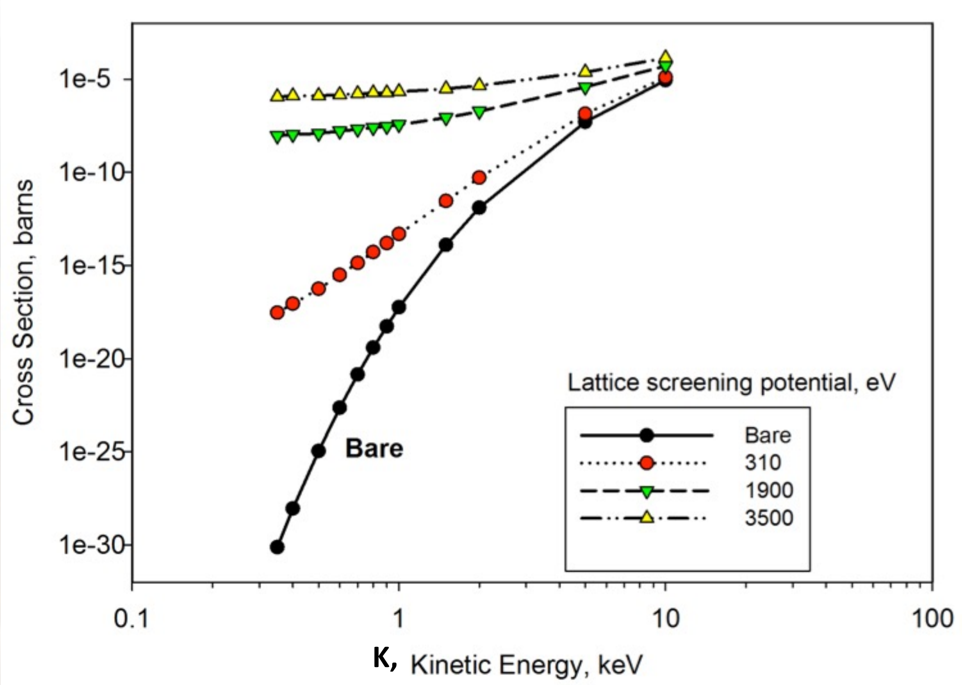


Glow Discharge or Plasma Ion source
X-ray and gamma photon source

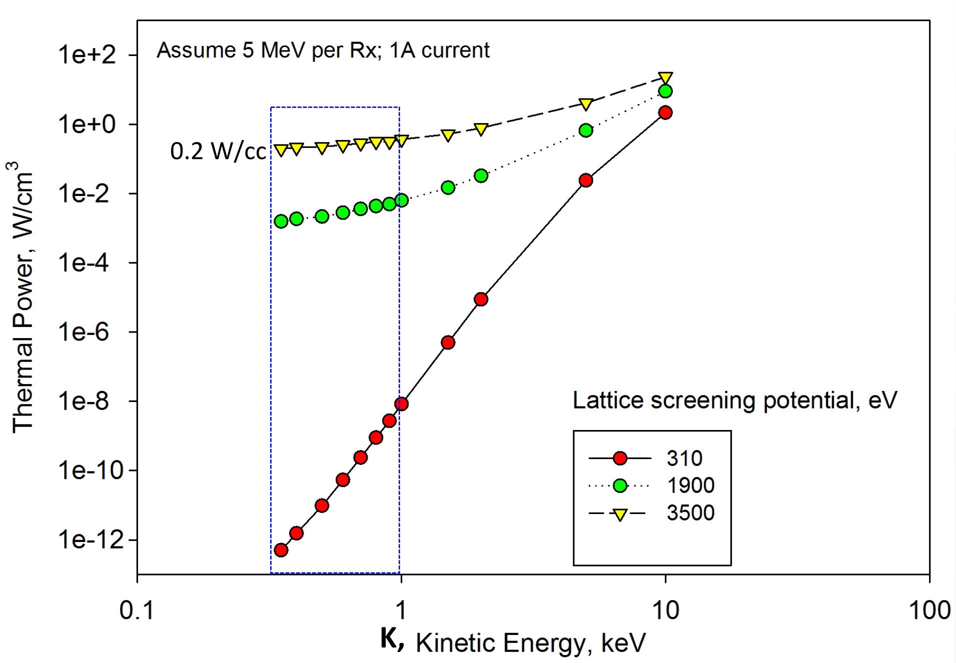
[1.] Calculations by V. Pines and M. Pines, NASA Advanced Energy Conversion Project

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

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

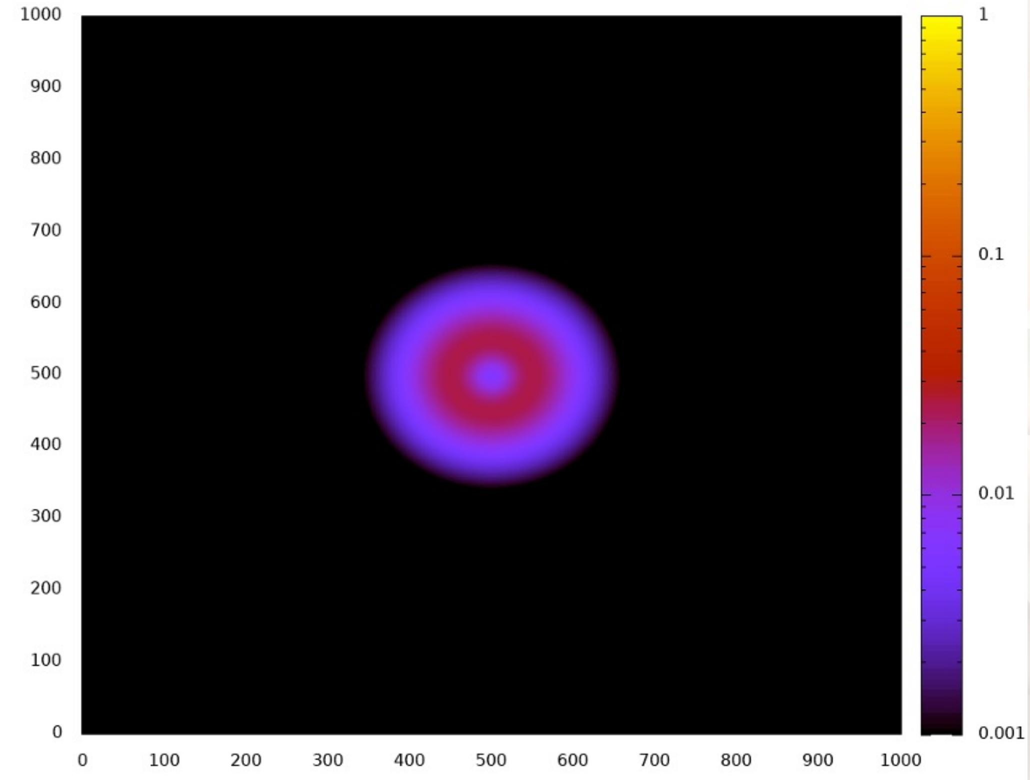
- ^{7}Be has astrophysical significance:
  - The decay rate in stellar cores effects the ^{8}B neutrino flux.
- It can be prepared terrestrially to study changes in half-life using the reaction:
  - ^{7}Li(p,n)^{7}Be, then
    - ^{7}Be decays by electron capture (EC) to ^{7}Li with a half-life, $t_{½}$, = 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

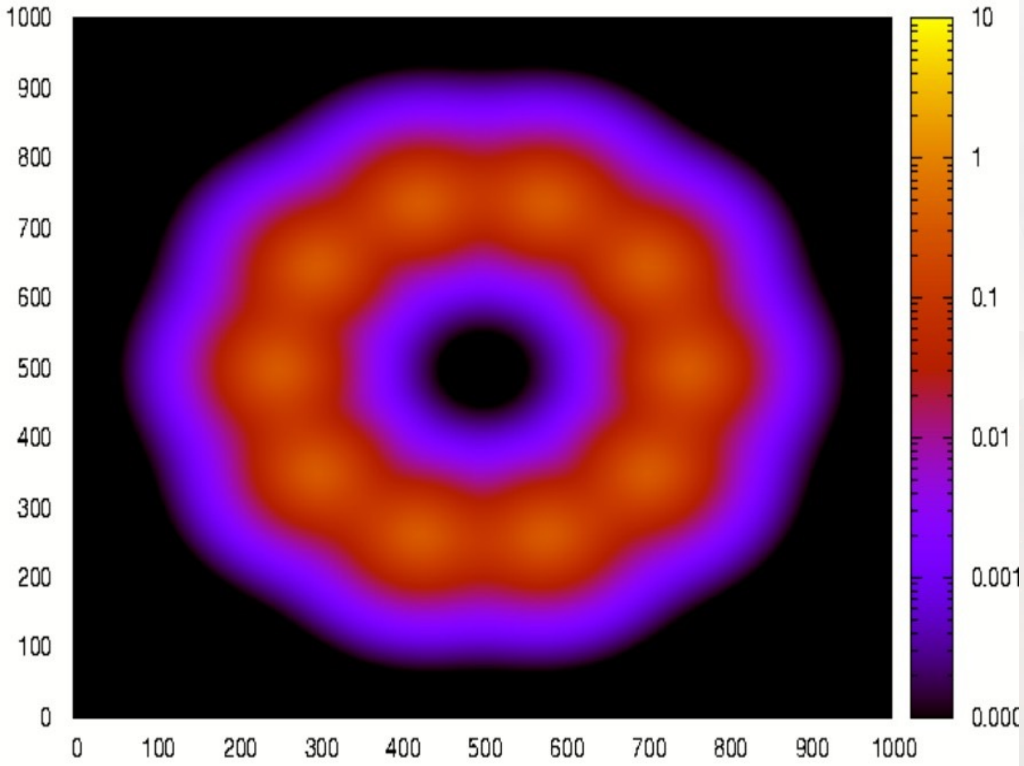
- Density Functional Theory (DFT) *e.g. Quantum Espresso, VASP, WIEN2K,etc*.
  - Solve the approximate Schrödinger equation in a solid lattice
  - Provides band structure and local electron density
  - Can calculate complex, inhomogeneous lattices and interfaces
  - Can incorporate external EM fields
- 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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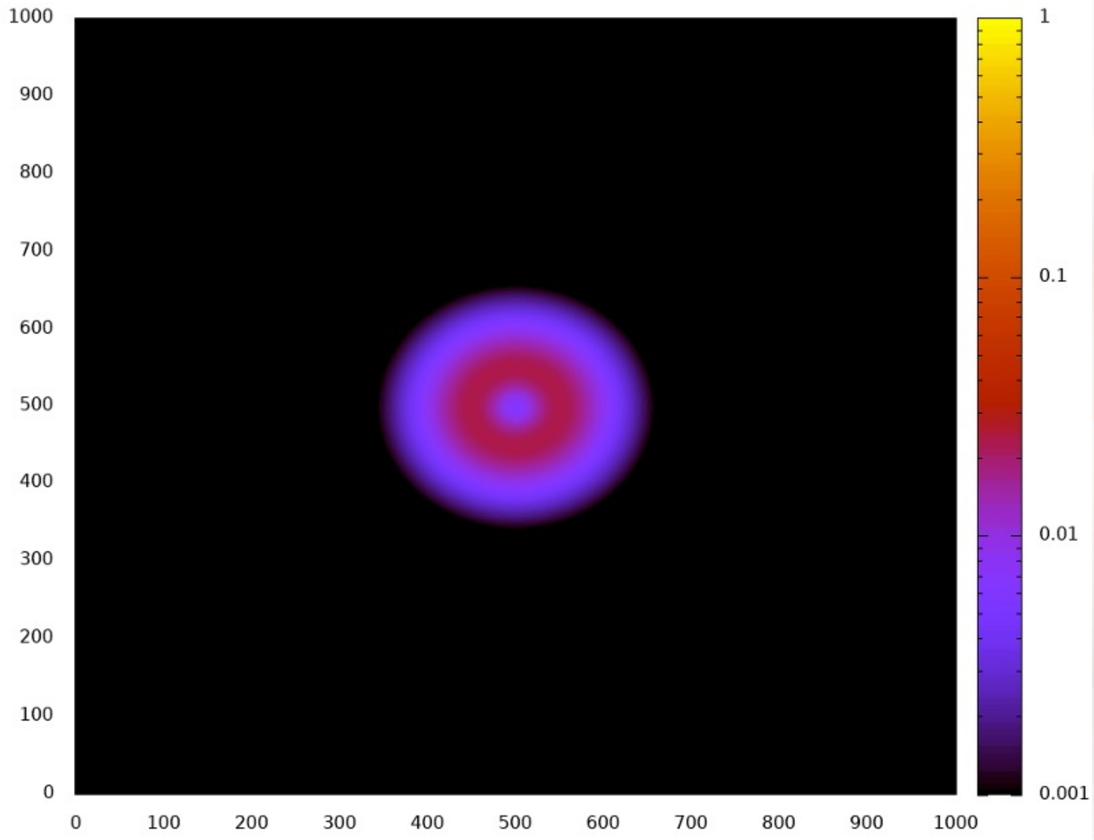
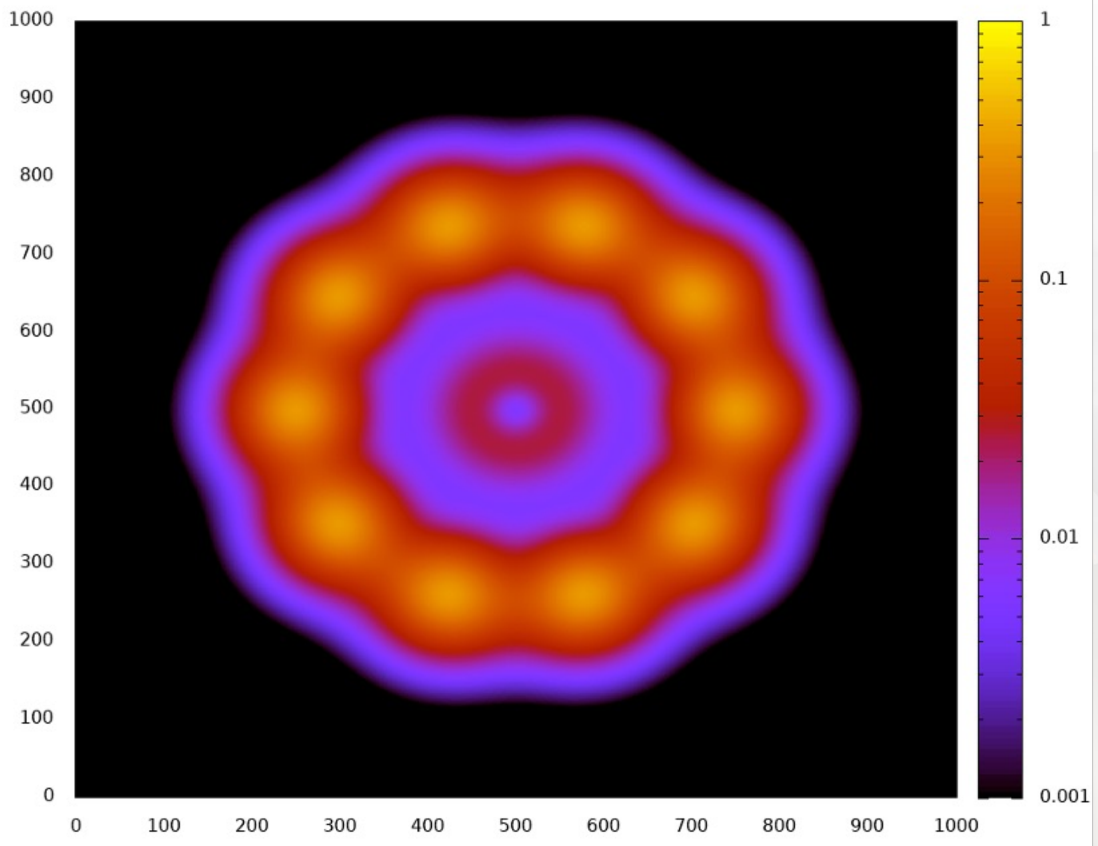
1 % decrease in electron cloud volume



Bare Be



Be embedded within C_{60} Fullerene "buckyball"

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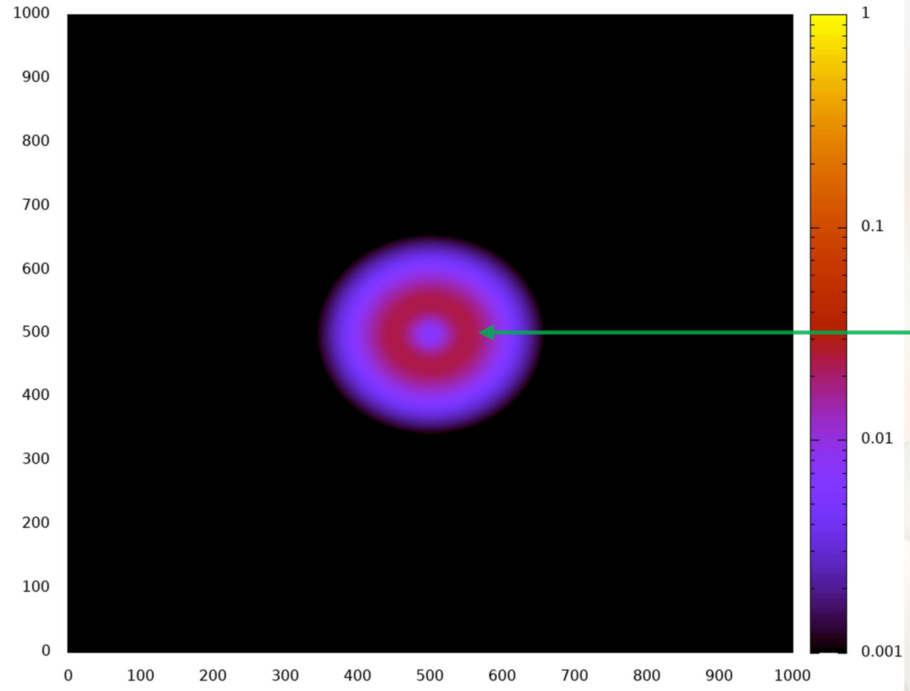
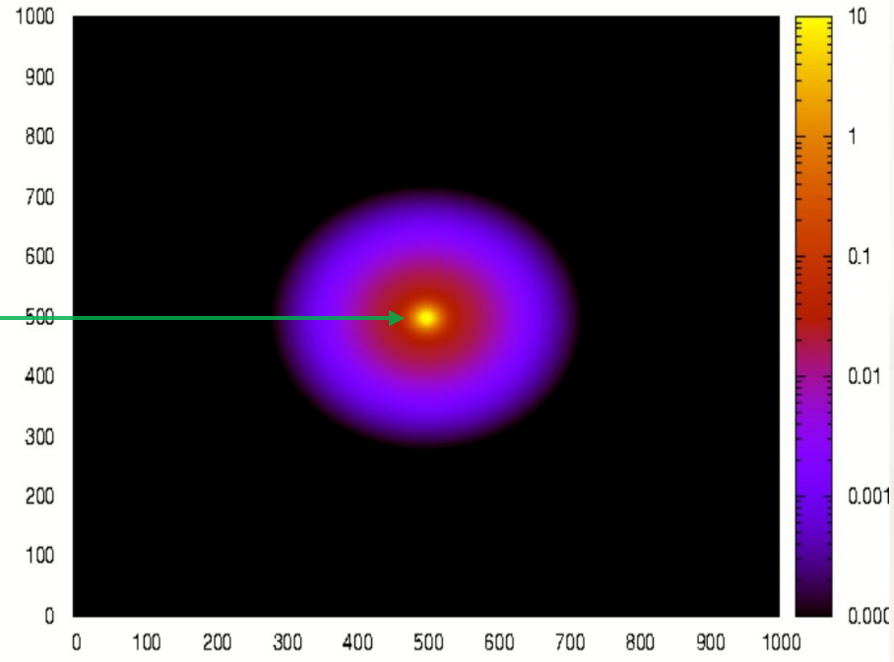
Comparison of Be $2s^2$ *and* $1s^2\,2s^2$ *electron densities*



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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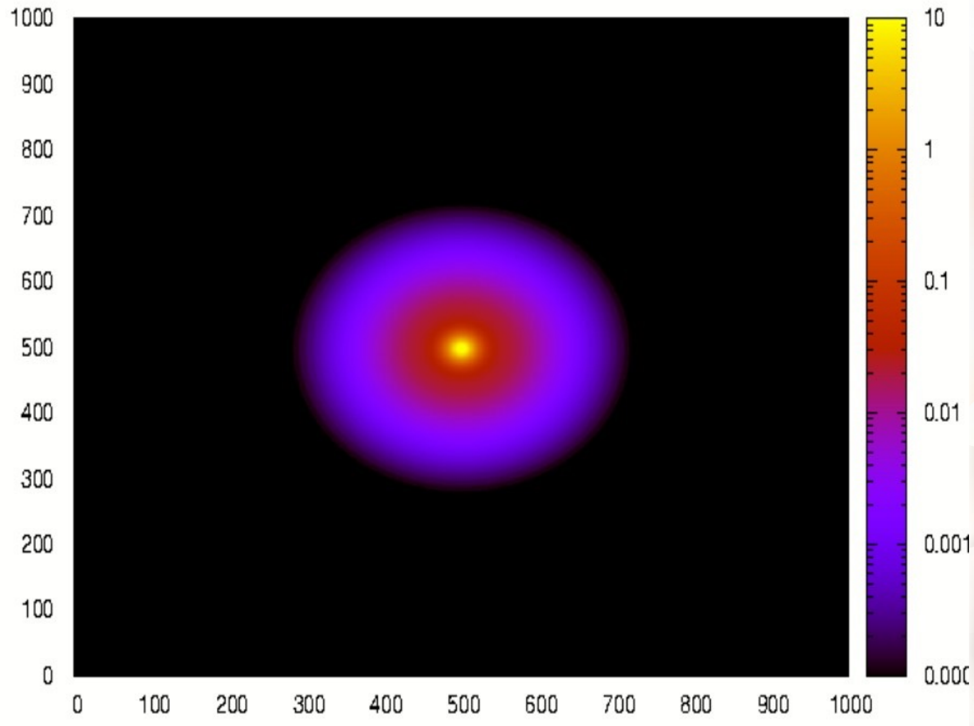
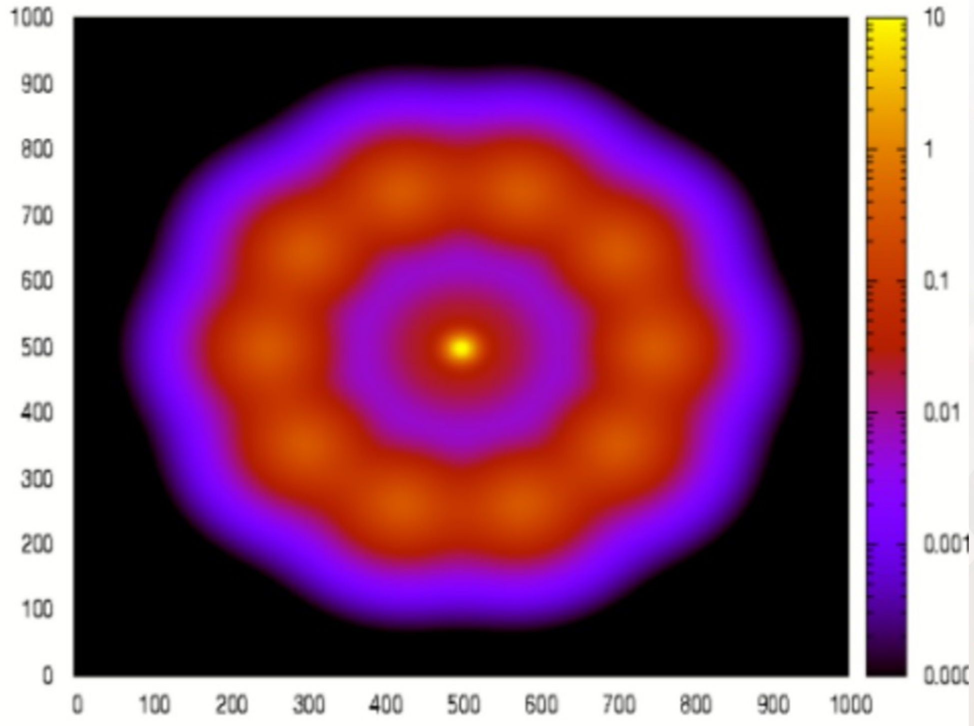
.1% decrease in electron density, but



Bare Be



Be embedded in C_{60}

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

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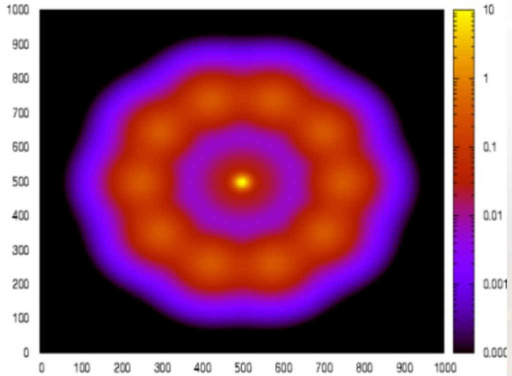

Be embedded in C_{60}

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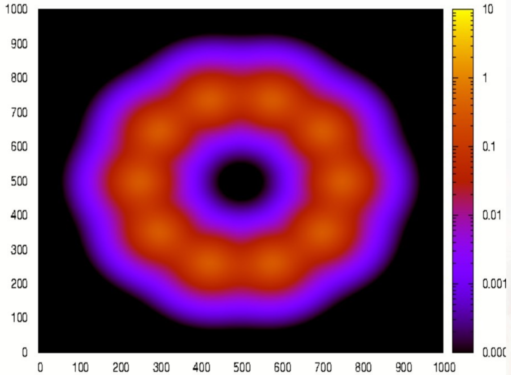
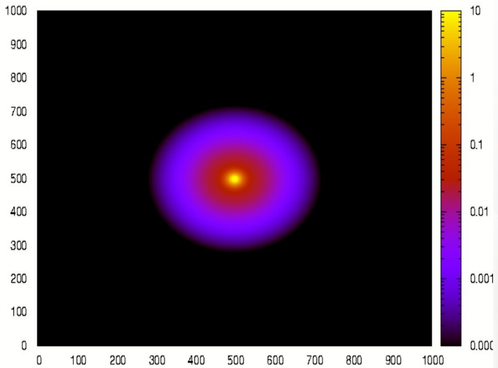


C_{60} alone

–



Be alone

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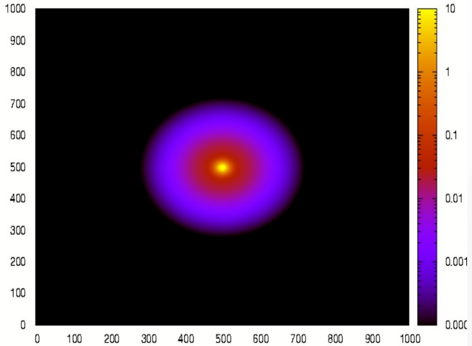
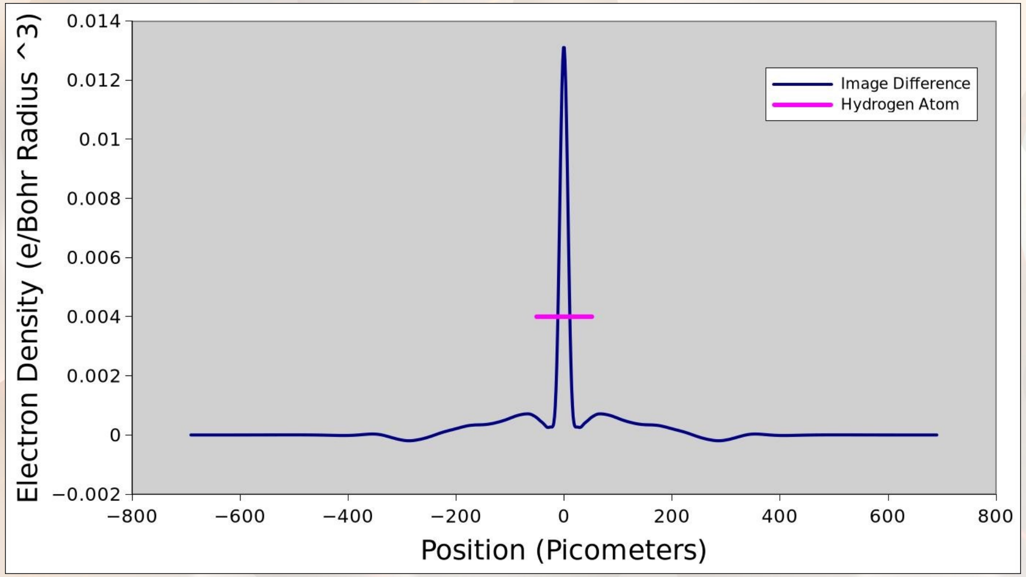


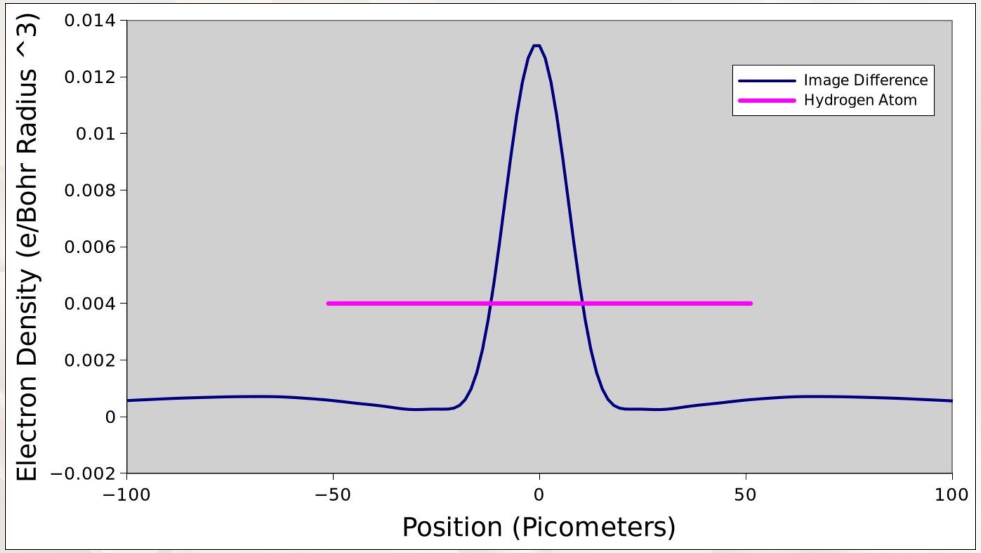
.1 % Be compression



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)

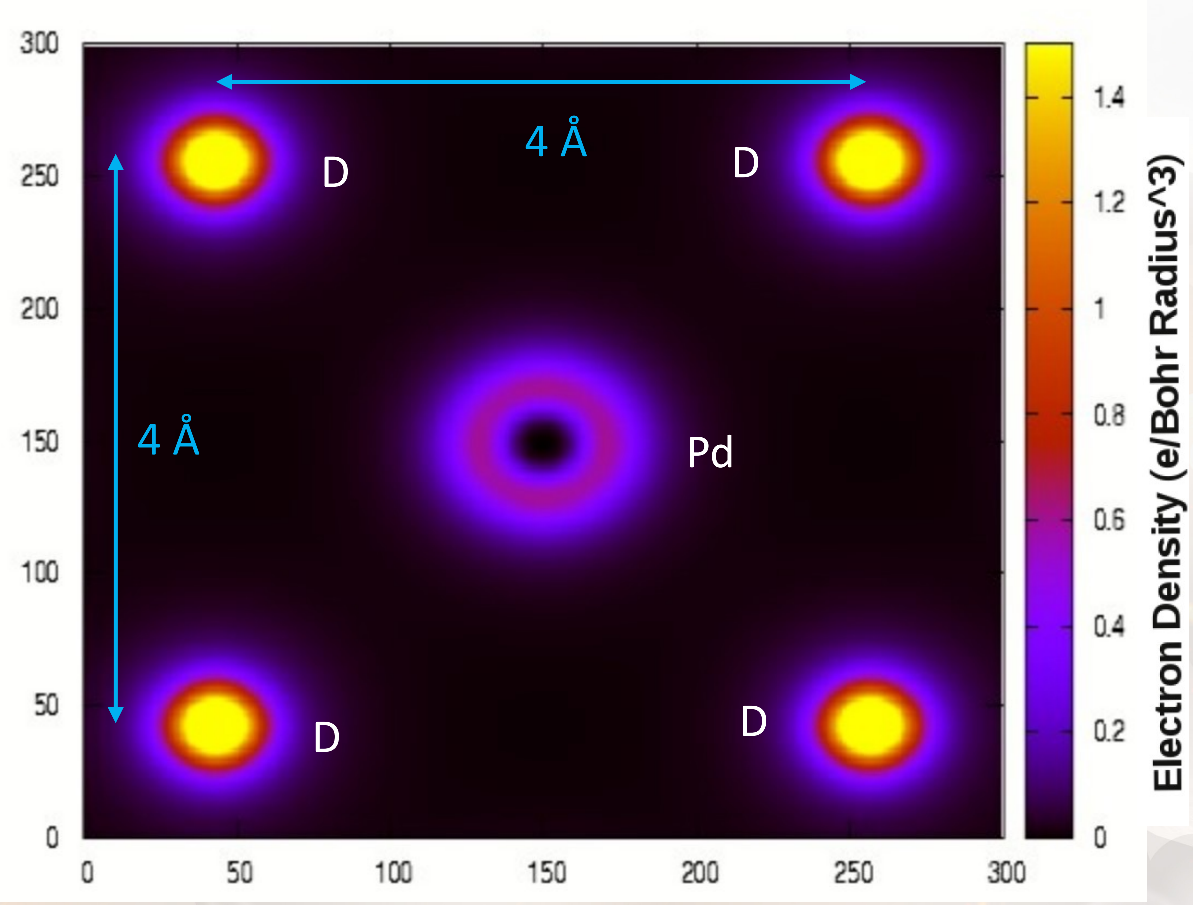


Closeup Be electron density

Pd/D and Pd CaO Lattice Electron Densities

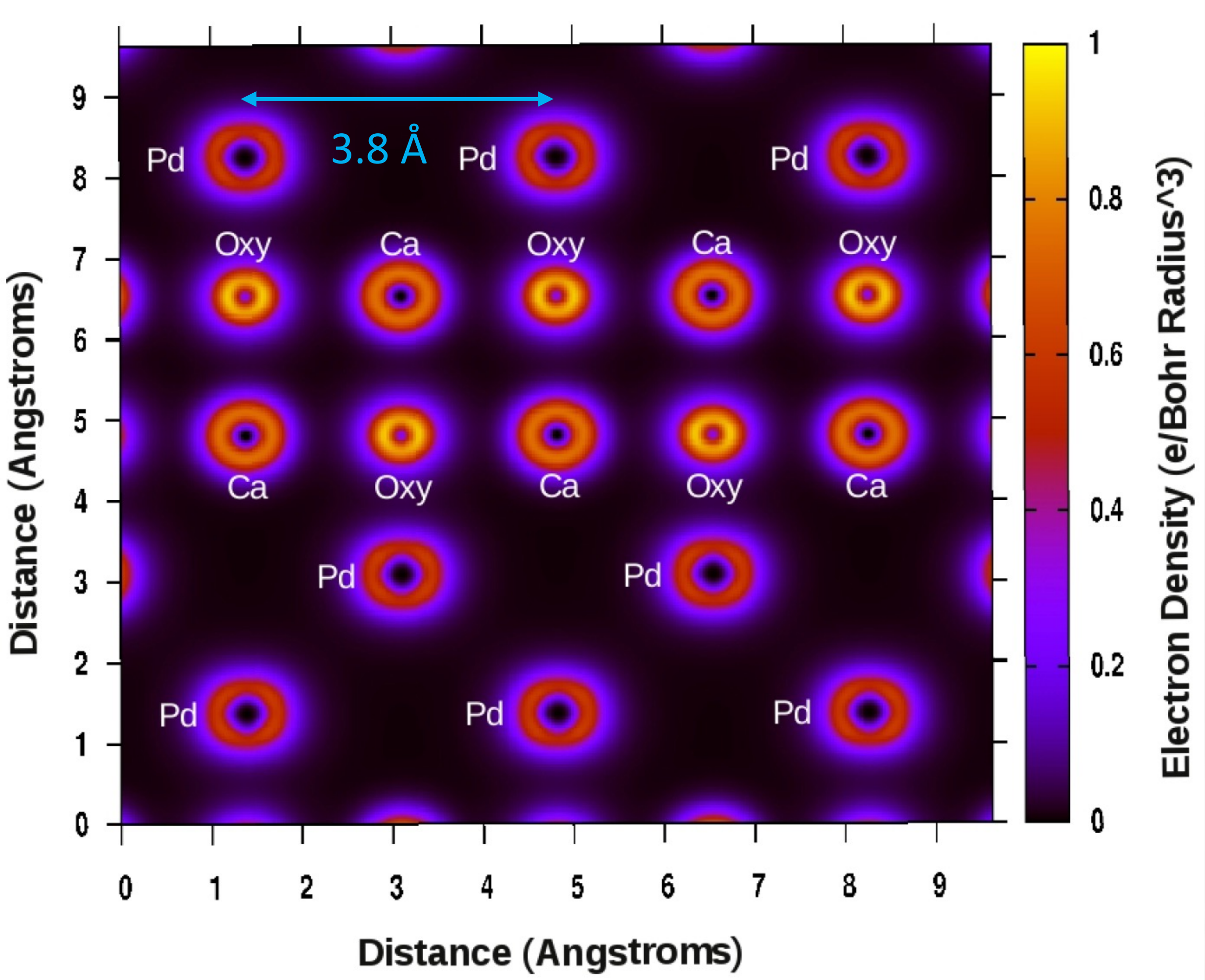
Just valence electrons

Modeling deuterium motion



Palladium Deuteride in SAV

Modeling induced ferromagnetism



Pd CaO Interface

Conclusion

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- 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

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In memorium of Dr. Marianna Pines