Electron Screened and Enhanced Nuclear Reactions

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Outline

1. Electron Screening, $U_e$
   - Astrophysics
   - Laboratory Astrophysics
   - 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, \( \approx 10^{23} \text{ e}^{-/\text{cm}^3} \)
   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

\( ^7\text{Be}_4 \) has astrophysical significance

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

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 \(^7\text{Be} \) at the solar core and the \(^8\text{B} \) neutrino flux.

Experiments diverge from theory below 6 keV

\( d(d,n)^3\text{He} \) fusion cross-section

Without screening

Pd Lattice Screening Potential Calculation\(^1\)

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

**Calculations by V. Pines and M. Pines, NASA Advanced Energy Conversion Project**
Comparison of Lattice vs. Deep Screening \(^1\).

How to increase deep screening?

![Graphs showing comparison of Lattice vs. Deep Screening](image)

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
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, $t_{1/2} = 53.12$ days
    - $\approx 10.4\%$ probability $^7$Be decays to the first $^7$Li excited state $3/2^{-}$
      - emitting 477.6 keV $\gamma$-ray photon.
- A 0.8% change in $^7$Be $t_{1/2}$ 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, $^4\text{Be}$) 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

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

Higher electron density calculated at nucleus by including both Be shells!
Be & Embedded Be, using Be 1s² 2s² orbitals

.1% decrease in electron density, but
Electron Density Within a Bohr radius \((5.3 \times 10^{-11} \text{m})^3\) volume

- Be embedded in \(\text{C}_{60}\)
- \(\text{C}_{60}\) alone
- Be alone

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

Be nucleus is \(\approx .003 \text{ pm (}10^{-15} \text{ m})\)

Broad electron density after subtractions

Closeup Be electron density
Pd/D and Pd CaO Lattice Electron Densities

Just valence electrons

Modeling deuterium motion

Modeling induced ferromagnetism

Palladium Deuteride in SAV

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
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In memorium of Dr. Marianna Pines