Developing first-principles multi-component density functional theory with emphasis on applications for exotic matter and exotic quantum states

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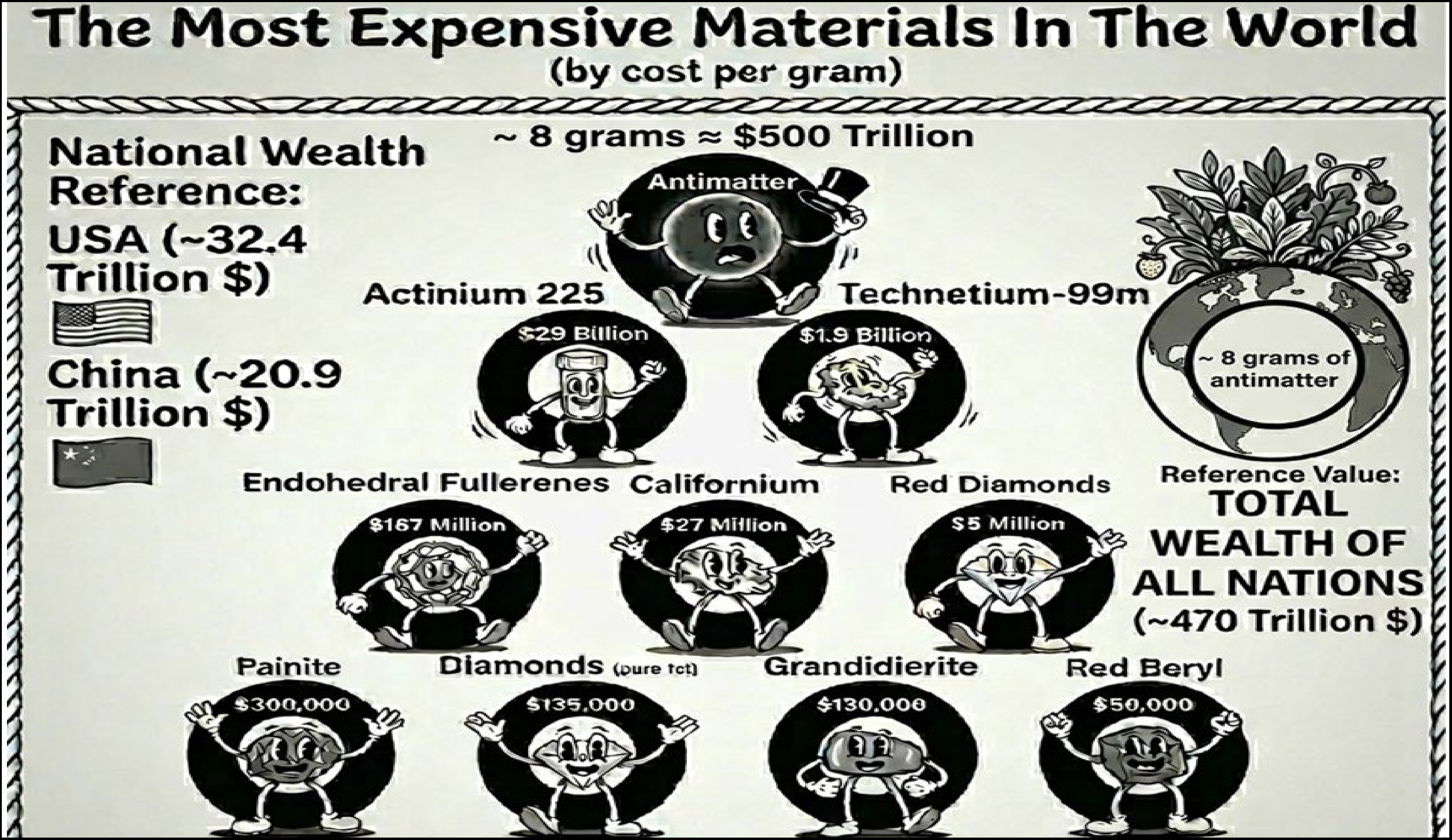
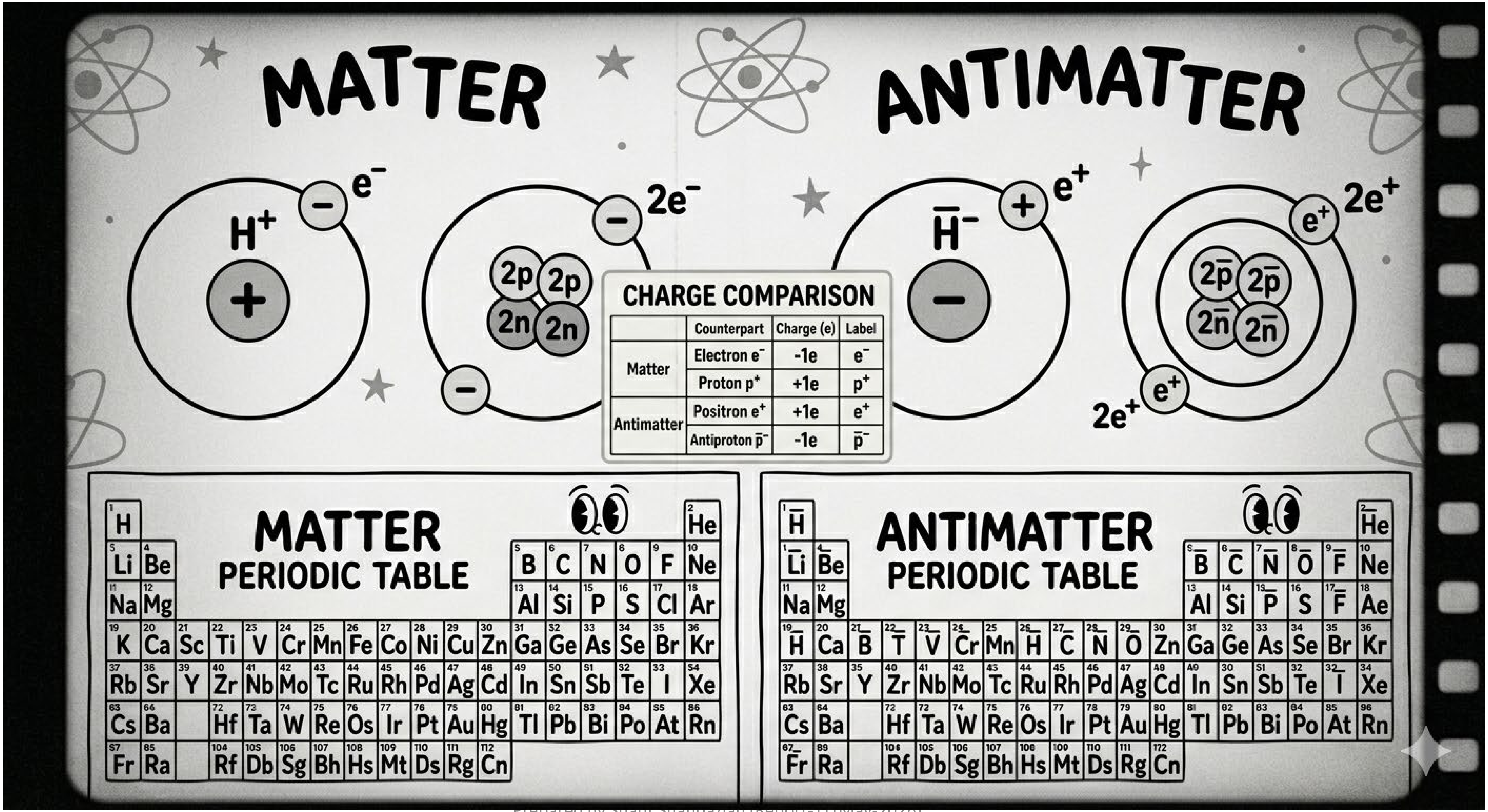
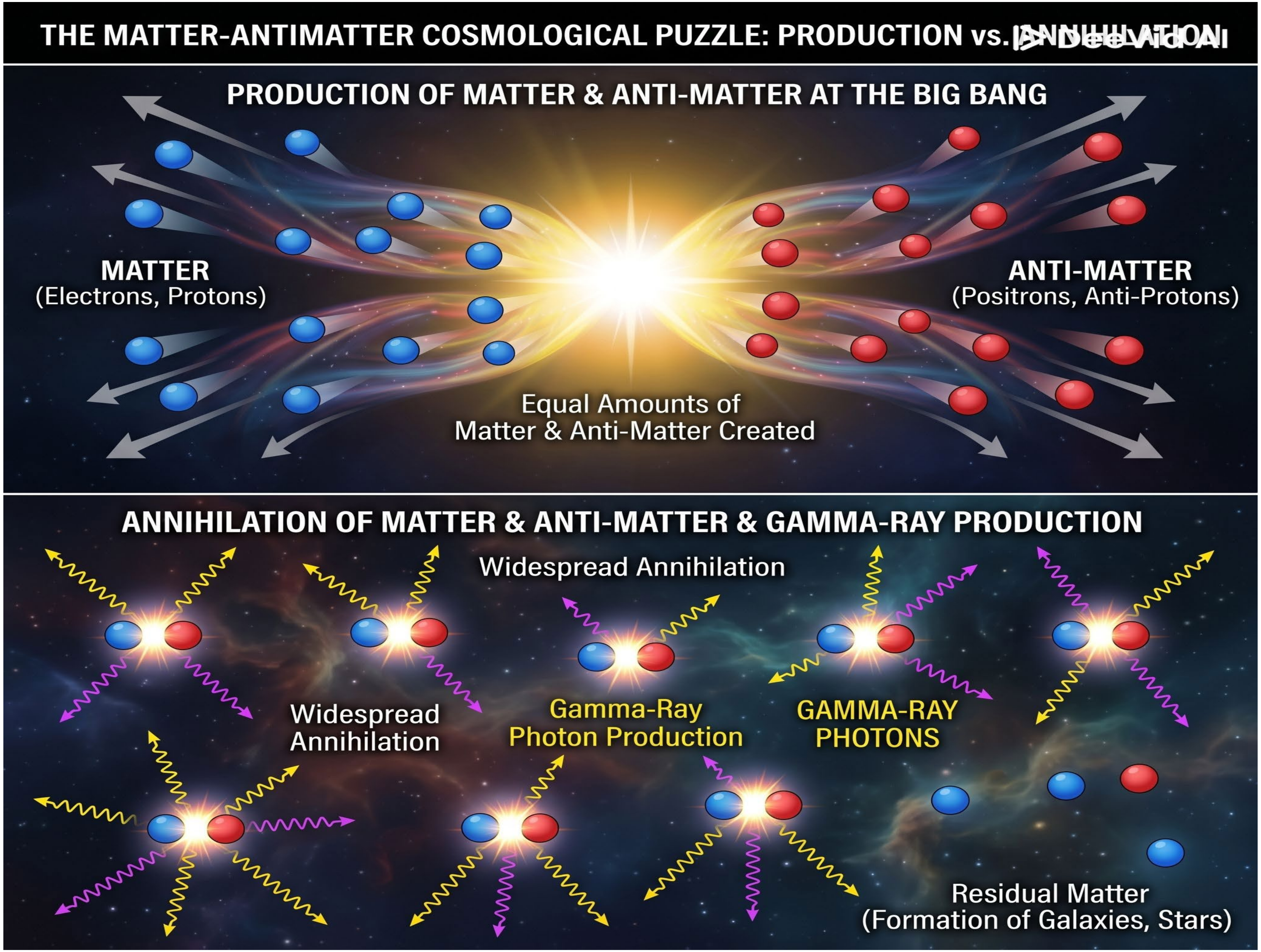
Prepared by Shant Shahbazian (Report-1) (May-2026)

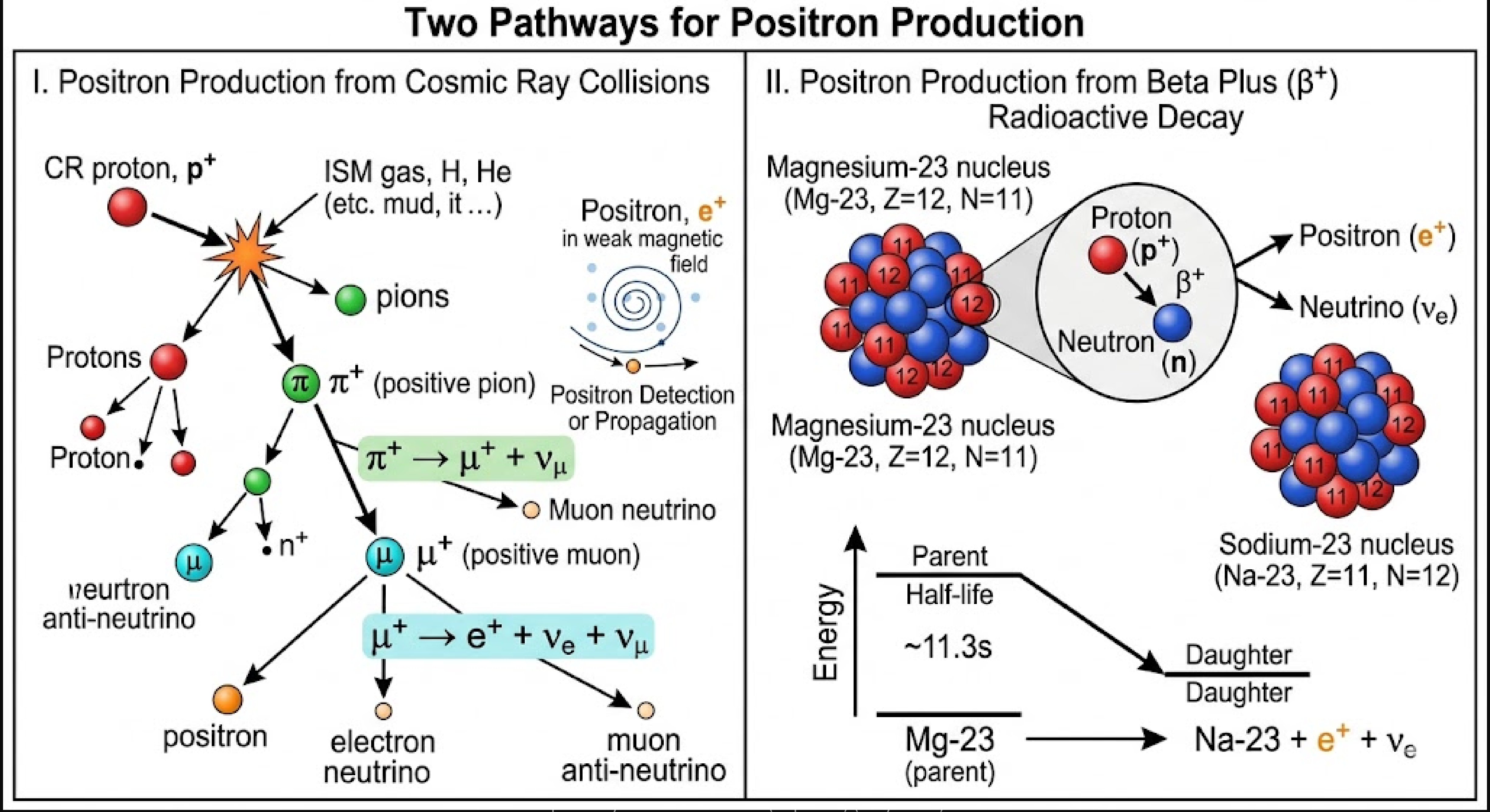
Summary of the project (25IRF-1C002)

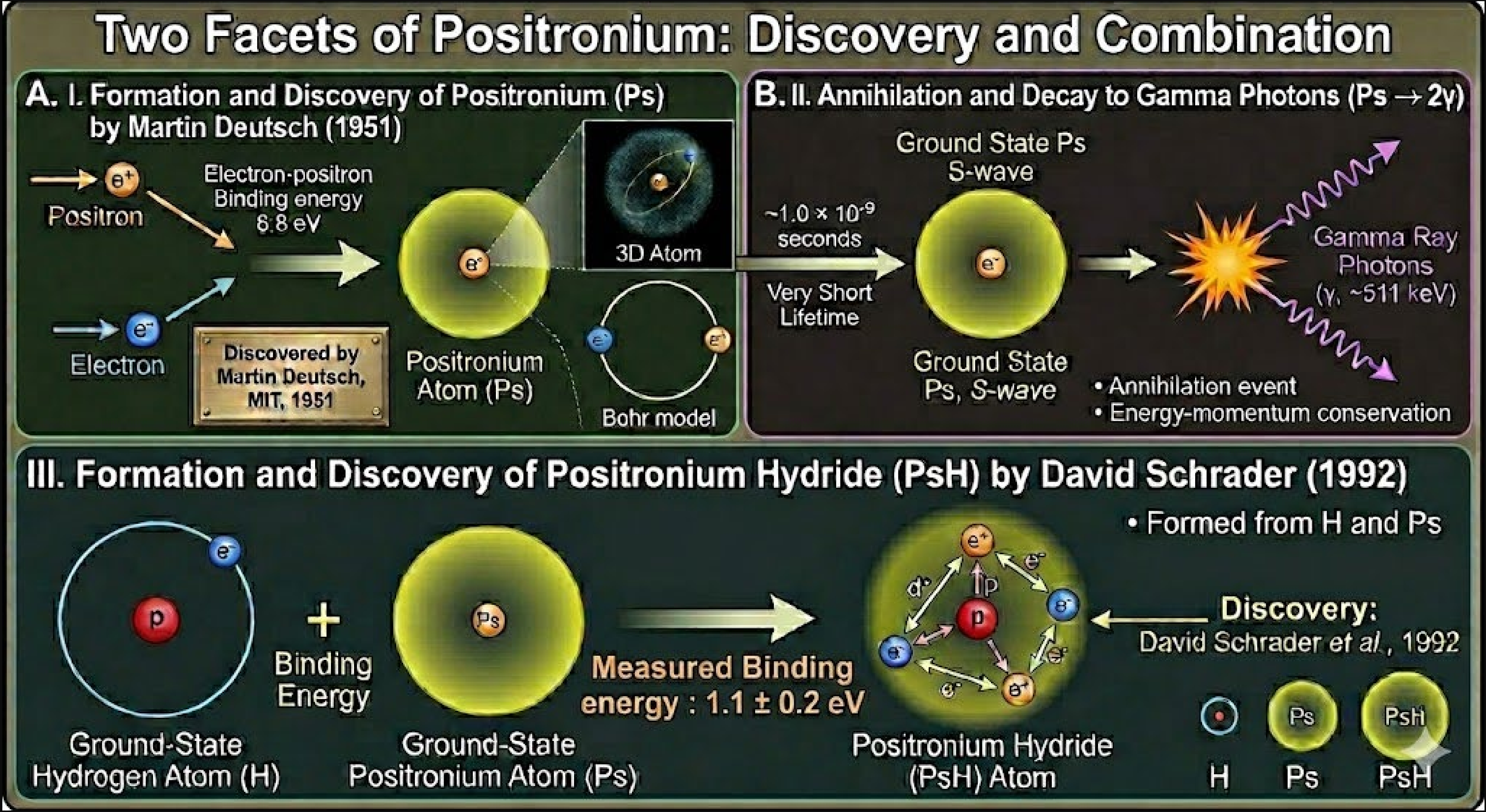
- **Date and place**: The project started on 27-Jun-2025 at the Division for Quantum Technologies, A. I. Alikhanyan National Laboratory (Yerevan Institute of Physics)
- **Group members**: Arshak Hovhannisyan, Hakob Khachatryan, and Qristinne Hovhannisyan
- **Main research themes**: 1) Quantum mechanics of few- and many-body systems, exactly solvable few-body quantum models, the internal structure of atoms and molecules composed simultaneously from matter and antimatter particles, superposed/delocalized quantum states of protons in molecules, quantum matter, e.g., metallic hydrogen, under extreme hydrostatic pressures, and 2) the many-body theory of reorganizable/deformable particles.
- **Publication**: *M. Goli, D. Bressanini, Sh. Shahbazian, Phys. Chem. Chem. Phys. "The two-positron gluic bond as a manifestation of 'super' van der Waals interactions"* 28, 11154 (2026)


The Most Expensive Materials In The World
(by cost per gram)
~ 8 grams ≈ $500 Trillion
Antimatter
National Wealth Reference:
USA (~32.4 Trillion $)
China (~20.9 Trillion $)
Actinium 225
$29 Billion
Technetium-99m
$1.9 Billion
~ 8 grams of antimatter
Endohedral Fullerenes
$167 Million
Californium
$27 Million
Red Diamonds
$5 Million
Reference Value:
TOTAL WEALTH OF ALL NATIONS
(~470 Trillion $)
Painite
$300,000
Diamonds (pure 1ct)
$135,000
Grandidierite
$130,000
Red Beryl
$50,000

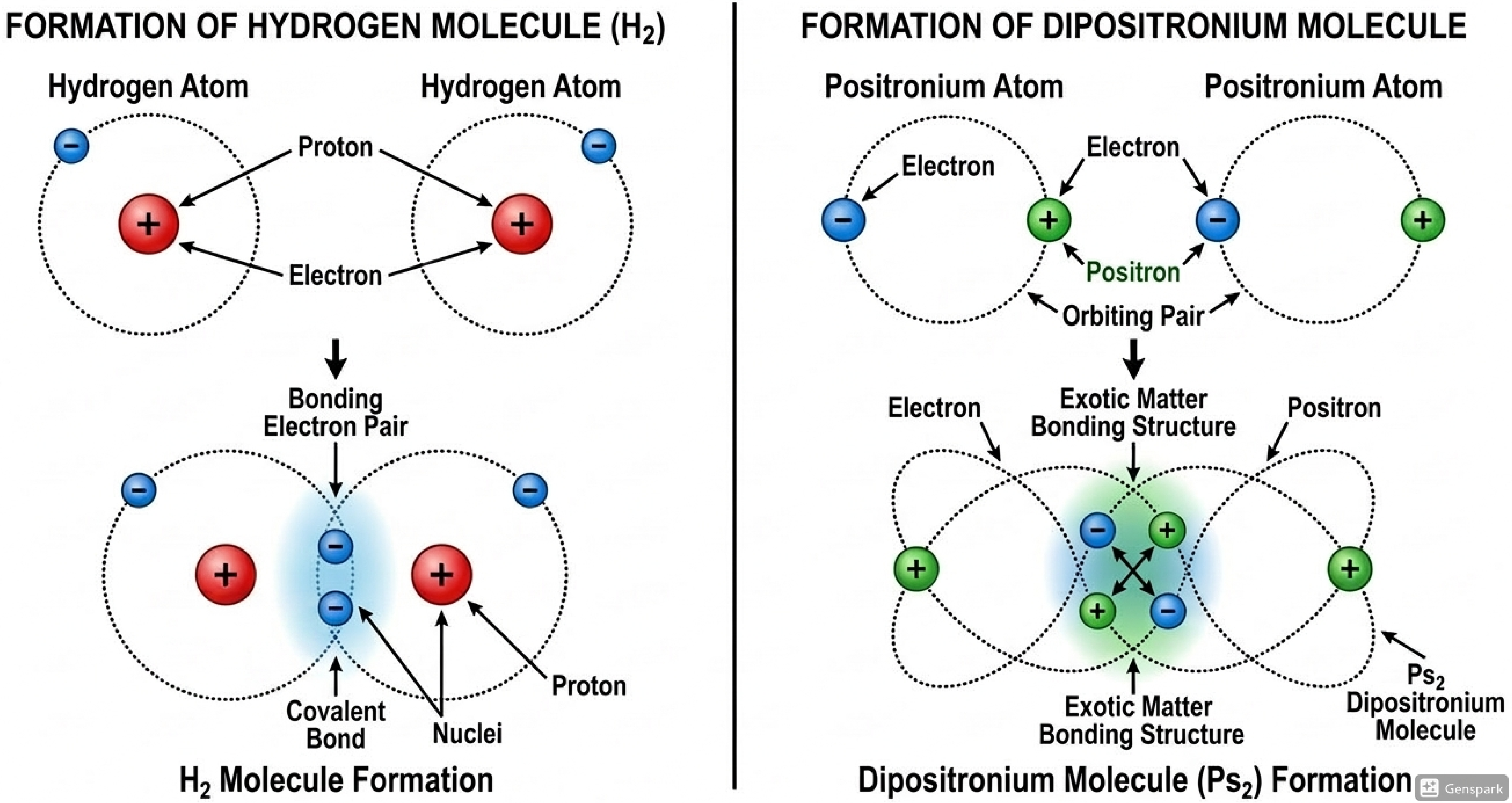

MATTER
ANTIMATTER
H+
e−
2e−
2p
2n
H̄−
e+
2e+
2p̄
2n̄
CHARGE COMPARISON
Counterpart | Charge (e) | Label
Matter | Electron e− | -1e | e−
Matter | Proton p+ | +1e | p+
Antimatter | Positron e+ | +1e | e+
Antimatter | Antiproton p̄− | -1e | p̄−
MATTER PERIODIC TABLE
ANTIMATTER PERIODIC TABLE

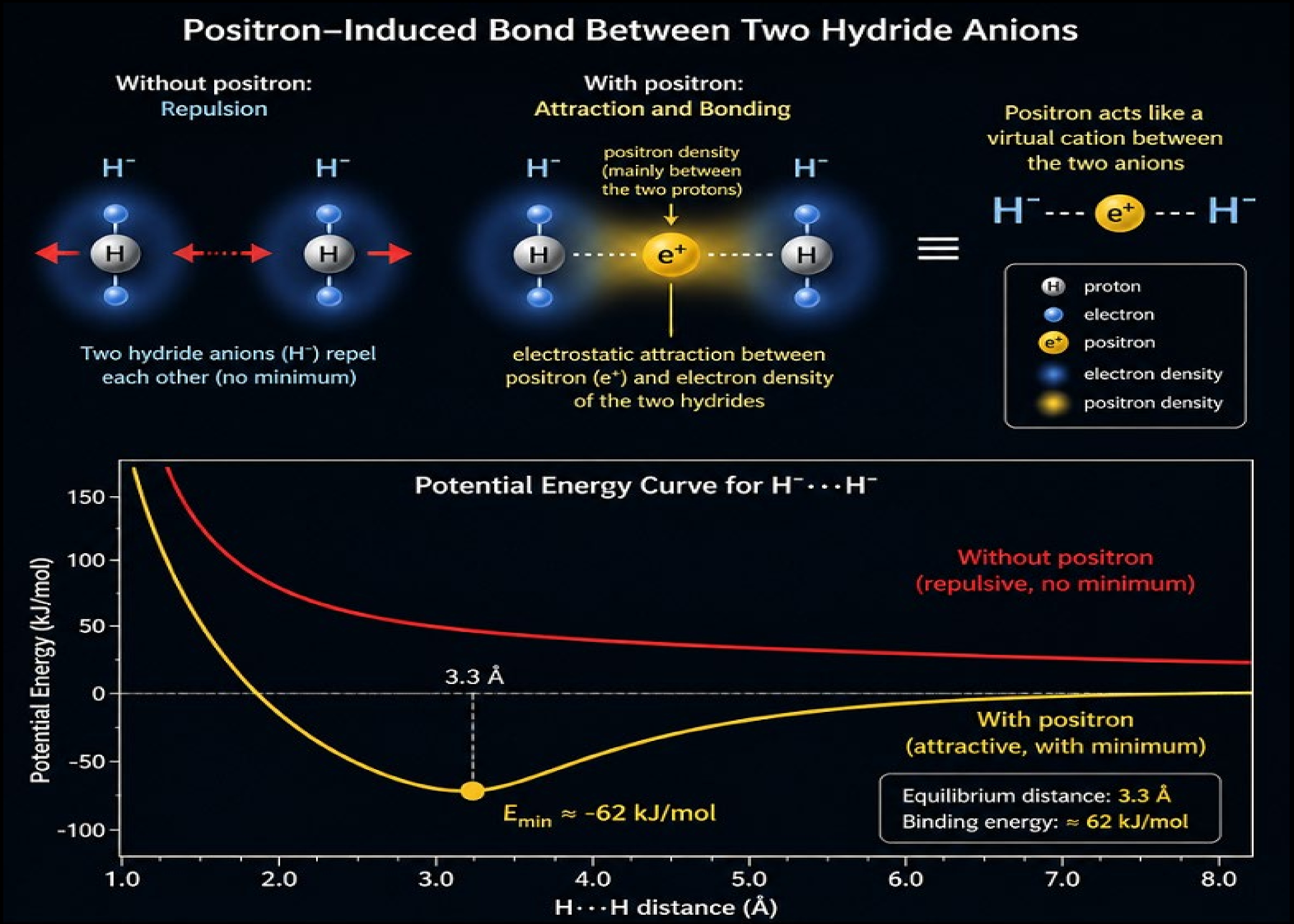

THE MATTER-ANTIMATTER COSMOLOGICAL PUZZLE: PRODUCTION vs. ANNIHILATION
DeeVid AI
PRODUCTION OF MATTER & ANTI-MATTER AT THE BIG BANG
MATTER
(Electrons, Protons)
ANTI-MATTER
(Positrons, Anti-Protons)
Equal Amounts of
Matter & Anti-Matter Created
ANNIHILATION OF MATTER & ANTI-MATTER & GAMMA-RAY PRODUCTION
Widespread Annihilation
Widespread
Annihilation
Gamma-Ray
Photon Production
GAMMA-RAY
PHOTONS
Residual Matter
(Formation of Galaxies, Stars)


Two Pathways for Positron Production
I. Positron Production from Cosmic Ray Collisions
CR proton, p+
ISM gas, H, He
(etc. mud, it ...)
pions
Positron, e+
in weak magnetic field
Positron Detection or Propagation
Protons
Proton
π
π+ (positive pion)
π+ → μ+ + νμ
Muon neutrino
n+
μ
neurtron anti-neutrino
μ+ (positive muon)
μ+ → e+ + νe + νμ
positron
electron neutrino
muon anti-neutrino
II. Positron Production from Beta Plus (β+) Radioactive Decay
Magnesium-23 nucleus
(Mg-23, Z=12, N=11)
Proton
(p+)
β+
Neutron
(n)
Positron (e+)
Neutrino (νe)
Magnesium-23 nucleus
(Mg-23, Z=12, N=11)
Sodium-23 nucleus
(Na-23, Z=11, N=12)
Energy
Parent
Half-life
~11.3s
Daughter
Daughter
Mg-23
(parent)
Na-23 + e+ + νe

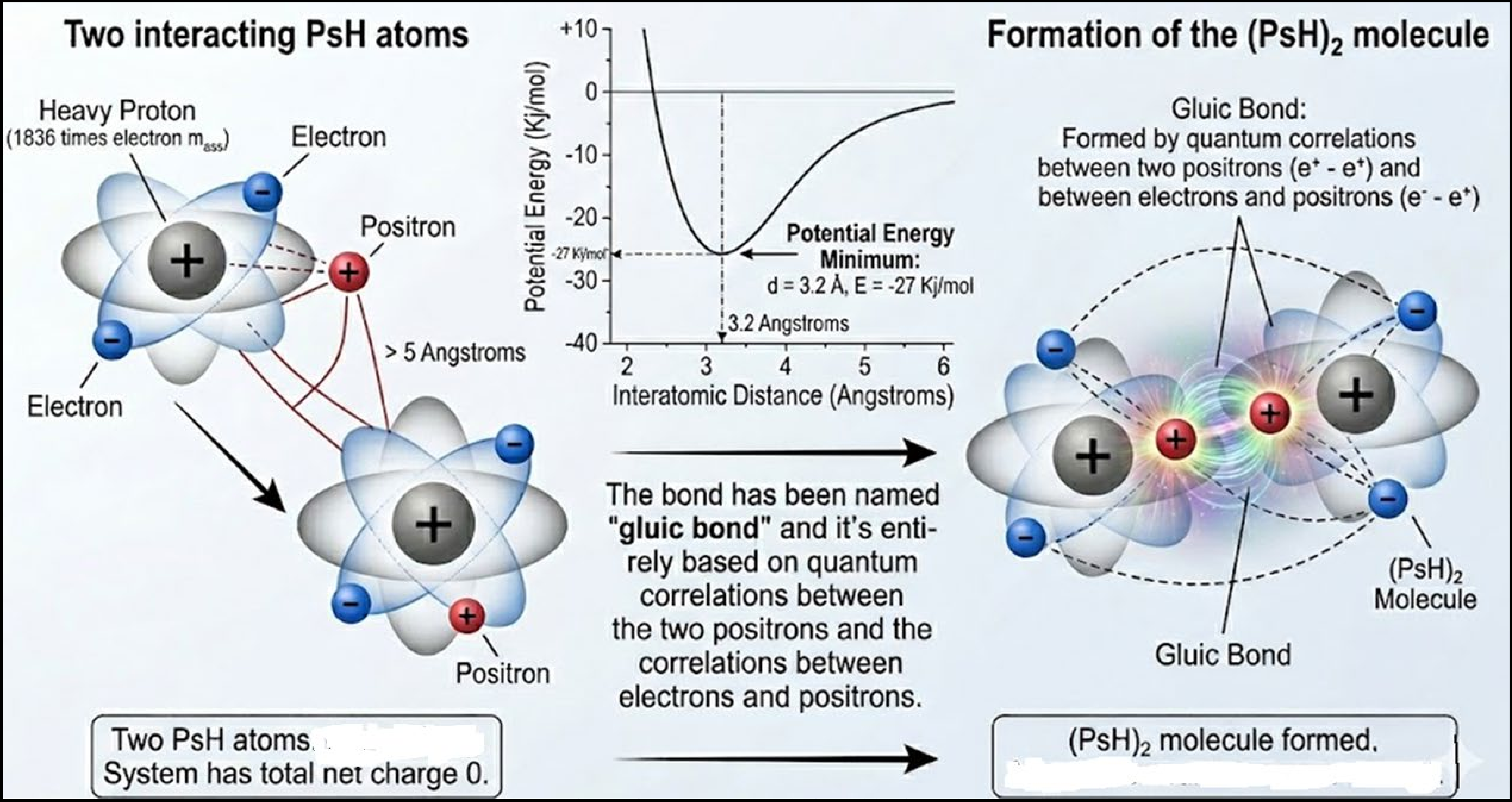

Two Facets of Positronium: Discovery and Combination
A. I. Formation and Discovery of Positronium (Ps) by Martin Deutsch (1951)
e+
Positron
Electron-positron Binding energy 6.8 eV
e-
Electron
Discovered by Martin Deutsch, MIT, 1951
e-
Positronium Atom (Ps)
3D Atom
e-
e+
Bohr model
B. II. Annihilation and Decay to Gamma Photons (Ps → 2γ)
~1.0 × 10-9 seconds
Very Short Lifetime
Ground State Ps S-wave
e-
Ground State Ps, S-wave
Gamma Ray Photons (γ, ~511 keV)
• Annihilation event
• Energy-momentum conservation
III. Formation and Discovery of Positronium Hydride (PsH) by David Schrader (1992)
• Formed from H and Ps
p
e-
Ground-State Hydrogen Atom (H)
+
Binding Energy
Ps
Ground-State Positronium Atom (Ps)
Measured Binding energy : 1.1 ± 0.2 eV
e+
e-
p
Positronium Hydride (PsH) Atom
Discovery:
David Schrader et al., 1992
H
Ps
PsH

COMPARISON OF MOLECULAR BONDING: COVALENT H_2 AND DIPOSITRONIUM

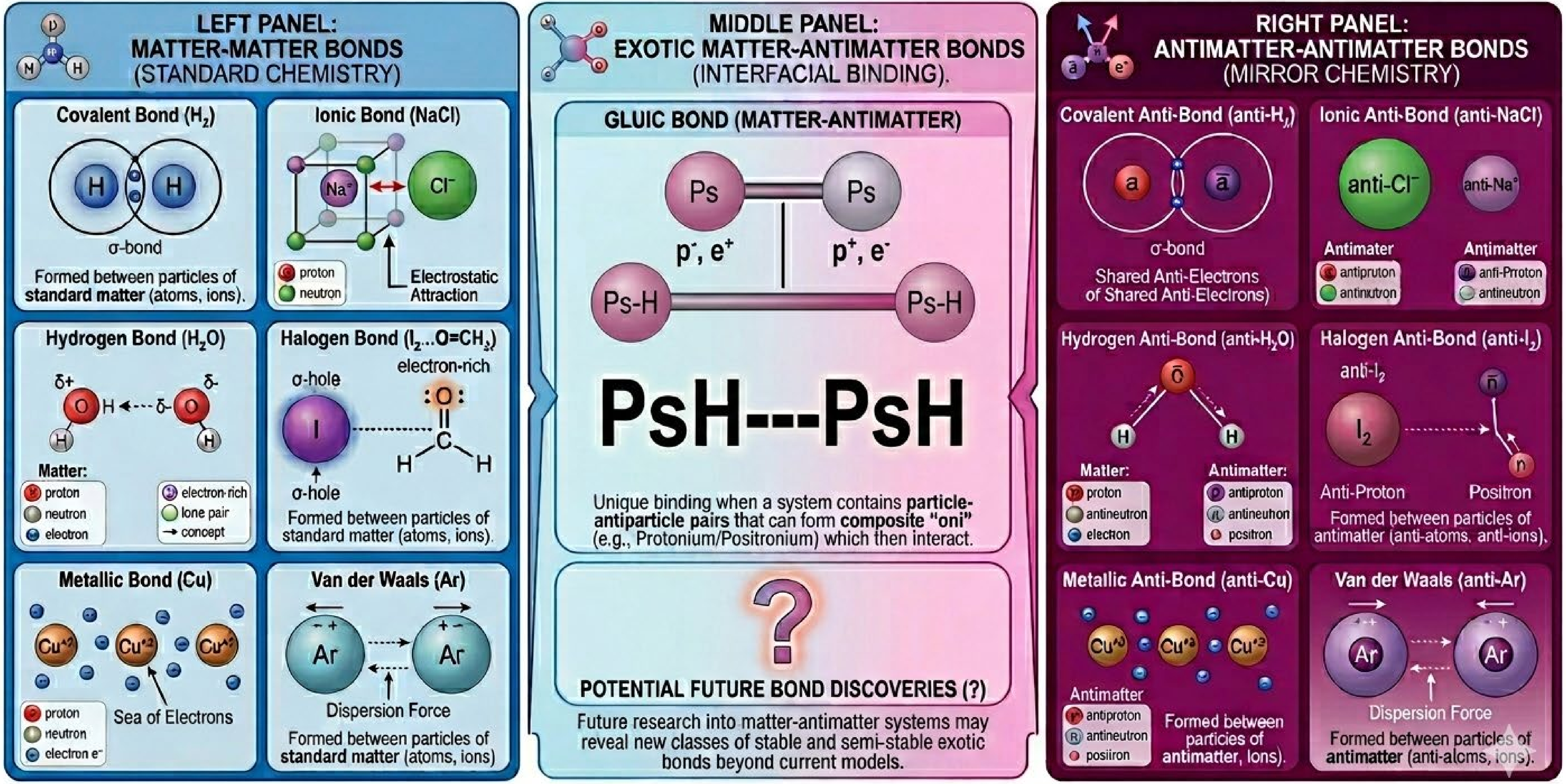




Positron–Induced Bond Between Two Hydride Anions
Without positron:
Repulsion
H^-
H^-
Two hydride anions (H^-) repel each other (no minimum)
With positron:
Attraction and Bonding
positron density (mainly between the two protons)
e^+
electrostatic attraction between positron (e^+) and electron density of the two hydrides
Positron acts like a virtual cation between the two anions
H^---- e^+ --- H^-
proton
electron
positron
electron density
positron density
Potential Energy Curve for $H^- \cdots H^-$
Potential Energy (kJ/mol)
H···H distance (Å)
Without positron (repulsive, no minimum)
With positron (attractive, with minimum)
3.3 Å
$E_{min} \approx -62$ kJ/mol
Equilibrium distance: 3.3 Å
Binding energy: ≈ 62 kJ/mol


Two interacting PsH atoms
Heavy Proton
(1836 times electron m_ass)
Electron
Positron
Electron
> 5 Angstroms
Positron
Two PsH atoms.
System has total net charge 0.
+10
0
-10
-20
-27 Kj/mol
-30
-40
Potential Energy (Kj/mol)
Potential Energy Minimum:
d = 3.2 Å, E = -27 Kj/mol
3.2 Angstroms
2
3
4
5
6
Interatomic Distance (Angstroms)
The bond has been named "gluic bond" and it's entirely based on quantum correlations between the two positrons and the correlations between electrons and positrons.
Formation of the $(PsH)_2$ molecule
Gluic Bond:
Formed by quantum correlations between two positrons (e^+ - e^+) and between electrons and positrons (e^- - e^+)
$(PsH)_2$ Molecule
Gluic Bond
$(PsH)_2$ molecule formed.

EXPLORING CHEMICAL BONDS ACROSS MATTER AND ANTIMATTER STATES.



Comparison of Standard and Exotic Binding Mechanisms

Thanks for your attention

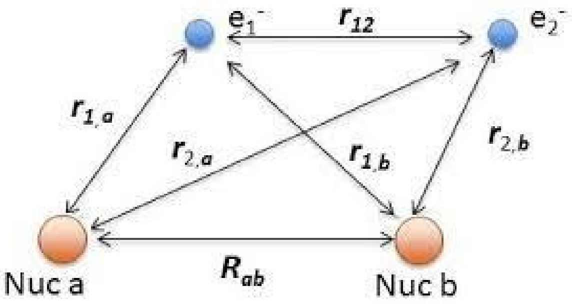
Supporting slides

The Heitler-London model on the origin of the homopolar covalent bonding

Interaction Between Neutral Atoms and Homopolar Binding According to Quantum Mechanics

W. Heitler and F. London

Z. Phys. **44**, 455 (1927)



$$\hat{H}_{H_2} = -\frac{1}{2m_e}\sum_{i=1}^{2}\nabla_i^2 + \frac{q_e^2}{|\vec{r}_1-\vec{r}_2|} + \sum_{X=a,b}\frac{q_e q_{nuc}}{|\vec{r}_i-\vec{R}_X|} + \frac{q_{nuc}^2}{|\vec{R}_a-\vec{R}_b|}$$

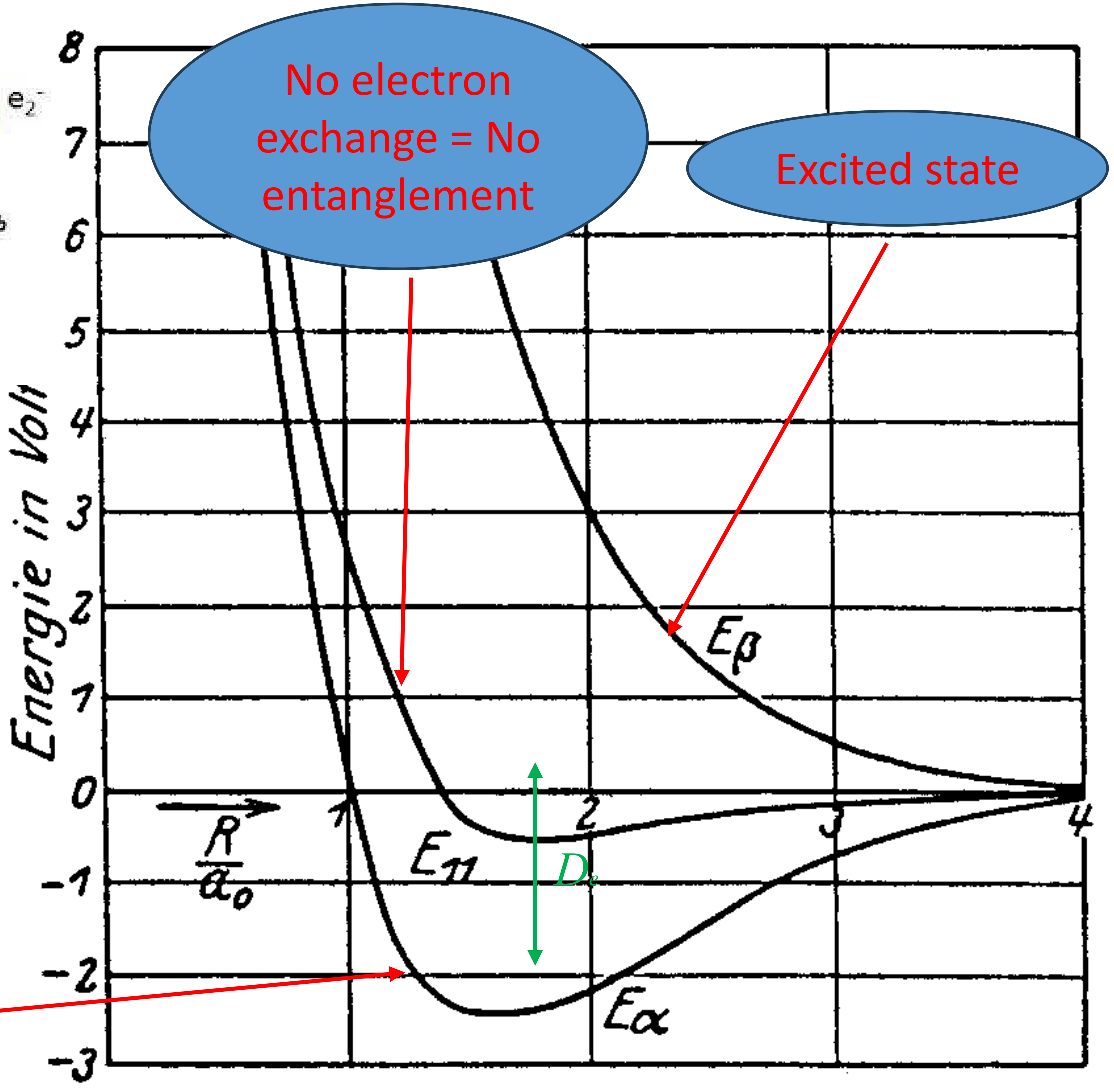
$$\hat{H}_{H_2}\Psi_{H_2}\left(\{\vec{r}_1,\vec{r}_2,\sigma_1,\sigma_1\};\{|\vec{R}_a-\vec{R}_b|\}\right) =$$

$$E_{H_2}\left(|\vec{R}_a-\vec{R}_b|\right)\Psi_{H_2}\left(\{\vec{r}_1,\vec{r}_2,\sigma_1,\sigma_1\};|\vec{R}_a-\vec{R}_b|\right)$$

Theory: D_e = 3.15 eV, R_e = 0.87 Å

Exp: D_e = 4.75 eV, R_e = 0.74 Å

Ground state



Z. Phys. 44, 455 (1927), Hinne Hettema, Quantum chemistry: Classic scientific papers, World Scientific, 2000.

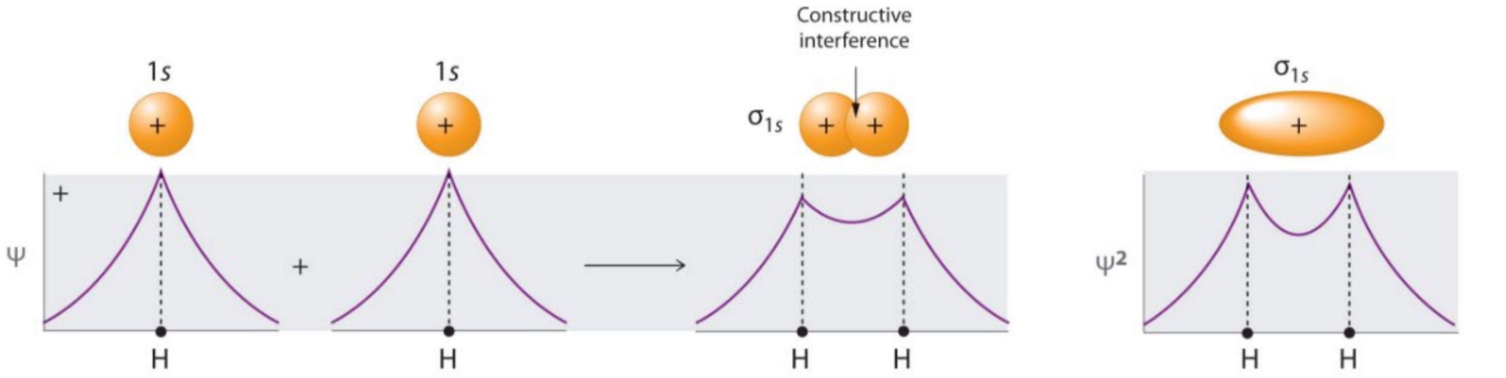
The Heitler-London (approximate) wavefunction and its ramifications

Ground state = covalent bond

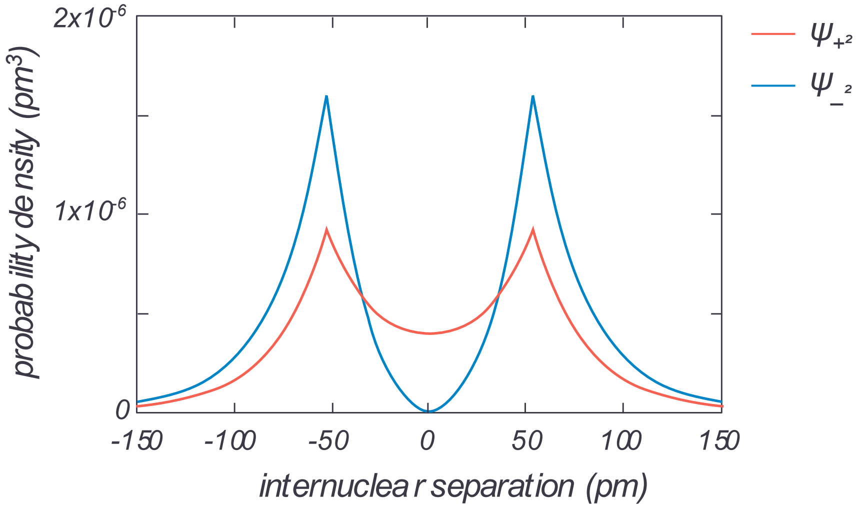
$$\frac{1s_a(1)1s_b(2) + 1s_a(2)1s_b(1)}{\sqrt{2}(1 + S_{12})^{1/2}} \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \alpha(2)\beta(1)]$$

Excited states = anti-bonding

$$\frac{1s_a(1)1s_b(2) - 1s_a(2)1s_b(1)}{\sqrt{2}(1 - S_{12})^{1/2}} \begin{cases} \alpha(1)\alpha(2) \\ 2^{-1/2}[\alpha(1)\beta(2) + \beta(1)\alpha(2)] \\ \beta(1)\beta(2) \end{cases}$$

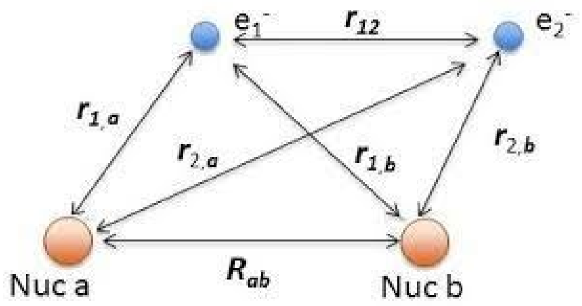


(a) Wave functions combined for σ_{1s} (b) Bonding probability density



(b)

Beyond the Heitler-London wavefunction: Approximate but practically exact wavefunctions



$$\xi_j = \frac{r_{aj} + r_{bj}}{R}, \qquad \eta_j = \frac{r_{aj} - r_{bj}}{R},$$

Dissociation energy of H_2 in the ground state (in cm^{-1}).

Year	Author	Experiment	Theory
1926	Witmer	35 000	
1927	Heitler–London		23 100
1933	James–Coolidge		36 104
1935	Beutler	36 116(6)	
1960	Kołos–Roothaan		36 113.5
1960	Herzberg–Monfils	**36 113.6(3)**	
1964	Kołos–Wolniewicz		**36 117.3**
1968	Kołos–Wolniewicz		**36 117.4**
1970	Herzberg	**36 118.3**	

$$\Psi = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) - \alpha(2)\beta(1)\right]\sum_i^M c_i\left(\Phi_i(1,2) + \Phi_i(2,1)\right),$$

$$\Phi_i(1,2) = \exp(-A\xi_1 - \bar{A}\xi_2)\xi_1^{n_i}\eta_1^{k_i}\xi_2^{m_i}\eta_2^{l_i}\left(\frac{2r_{12}}{R}\right)^{\mu_i}\cdot$$

$$\cdot\left(\exp(B\eta_1 + \bar{B}\eta_2) + (-1)^{k_i+l_i}\exp(-B\eta_1 - \bar{B}\eta_2)\right),$$

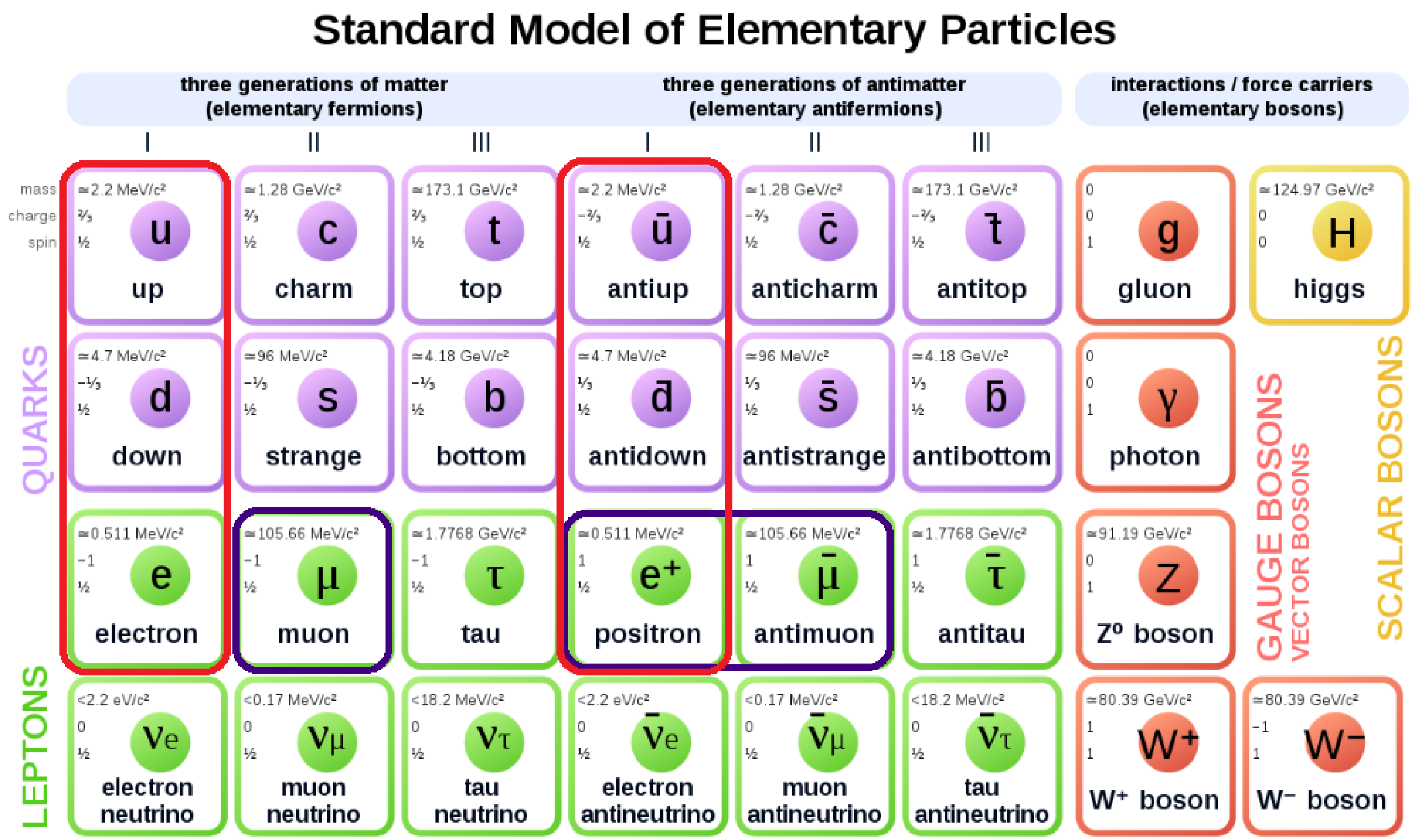
Sometimes the only way to answer a question is to solve the exact model numerically...

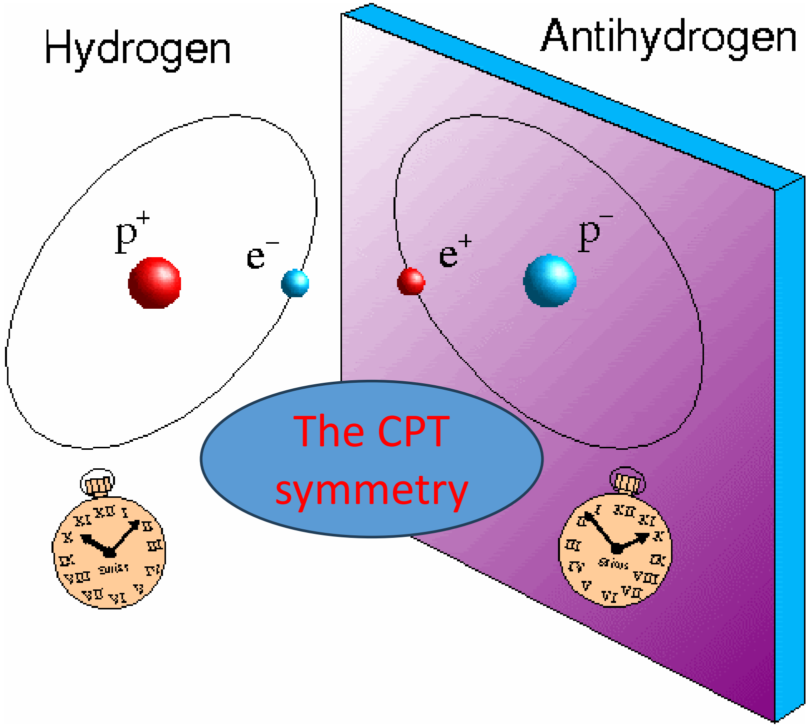
$c_i,\ A,\ \bar{A},\ B,\ \bar{B}$ are variational parameters

$n,\ k,\ l,\ m,\ \mu$ are integers

JCP 1, 825 (1933), RMP 32, 205 (1960), JCP 41, 3663 (1964), JCP 49, 404 (1968), Adv. Quantum Chem. 87, 1 (2023)

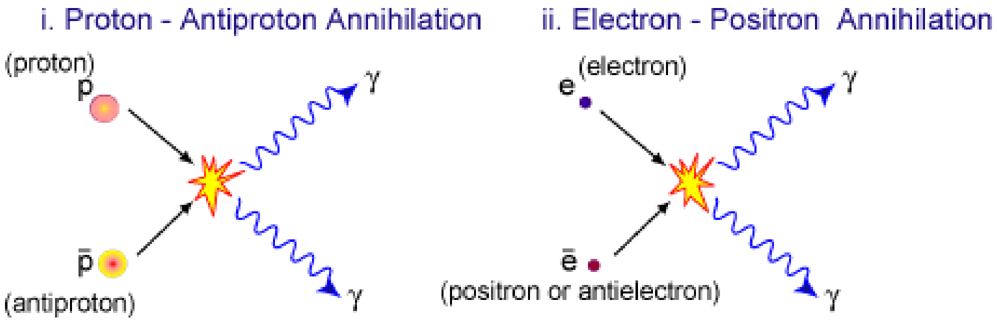
The mirror symmetry of matter and anti-matter





Maybe there is antichemistry somwhere,

and who knowns, maybe even antibiochemistry...



In each case the particle and its antiparticle annihilate each other, releasing a pair of high-energy gamma photons

Timeline of some important experiments on the anti-hydrogen atom

2002: cold antihydorgen atoms were first produced at CERN

2010: the first cold antihydrogen atoms were trapped successfully

2016: the spectrocopic 1s-2s transition frequency was meausred and it was demonstrated to be equal to that of the hydrogen atom's transition frequency within the error bars of the measurements

2023: it was demonstrated that antihydrogen falls in the gravitational field similar to hydrogen atom obaying Newton's gravitional law (no negative mass)

2025: the hyper-fine structure components of 1S-2S transitions was observed and was demonstrated to be equal to that of the hydrogen atom's transition frequency within the error bars of the measurements

As far as these experiments reveal until now, within the error bars of the measurments, there is no difference between properties of the hydrogen and antihydrogen atoms

Nature 419, 456 (2002), Nature 468, 673 (2010), Nature 541, 506 (2016), Nature 621, 716 (2023), Nature Phys. 21, 507 (2025)

The spectroscopy of the anti-hydrogen atom: 1S-2S transition

nature physics

Article

https://doi.org/10.1038/s41567-024-02712-9

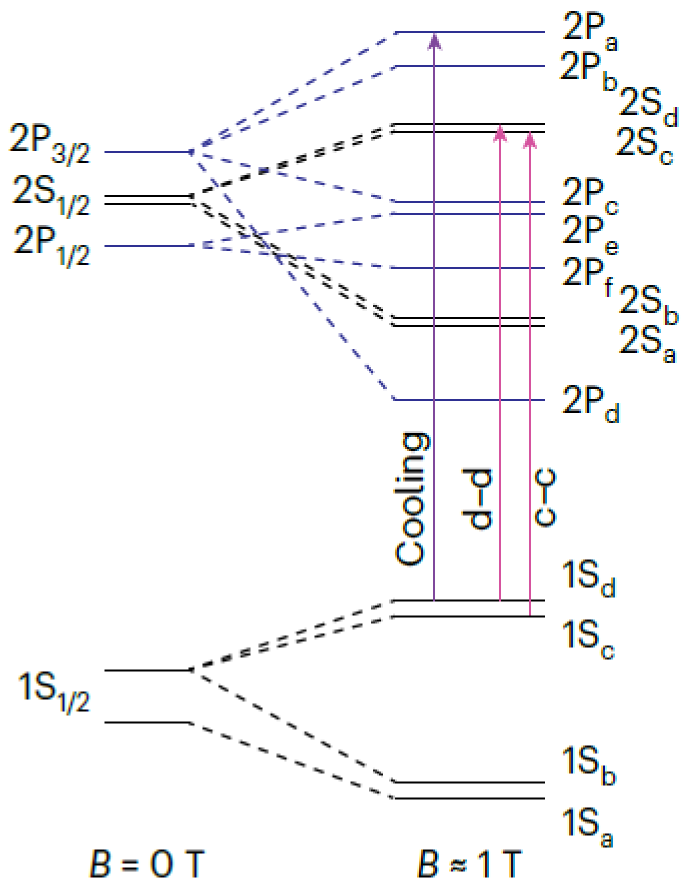
Precision spectroscopy of the hyperfine components of the 1S–2S transition in antihydrogen

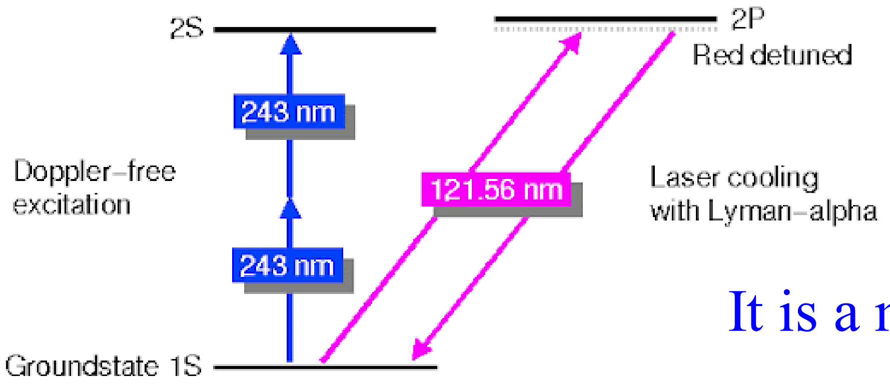
Received: 11 October 2022

Accepted: 14 October 2024

Published online: 17 January 2025

C. J. Baker[1], W. Bertsche[2,3], A. Capra[4], C. Carruth[5], C. L. Cesar[6], M. Charlton[1], A. Christensen[5], R. Collister[4], A. Cridland Mathad[1], S. Eriksson[1], A. Evans[7], N. Evetts[8], J. Fajans[5], T. Friesen[7], M. C. Fujiwara[4], D. R. Gill[4], P. Grandemange[4,7], P. Granum[9], J. S. Hangst[9], W. N. Hardy[8],

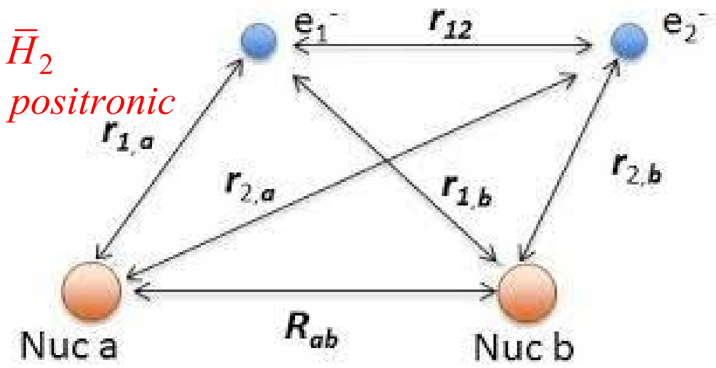




It is a matter of time to produce the first antiHydrogen molecule...

Mirror symmetry between covalent and "anti-covalent" bonds

$$\hat{H}^{H_2}_{elec}\Psi^{H_2}_{elec} = E^{H_2}_{e}\left(R_{ab}\right)\Psi^{H_2}_{elec} \qquad \hat{H}^{\bar{H}_2}_{positronic}\Psi^{\bar{H}_2}_{positronic} = E^{\bar{H}_2}_{positronic}\left(R_{ab}\right)\Psi^{\bar{H}_2}_{positronic}$$



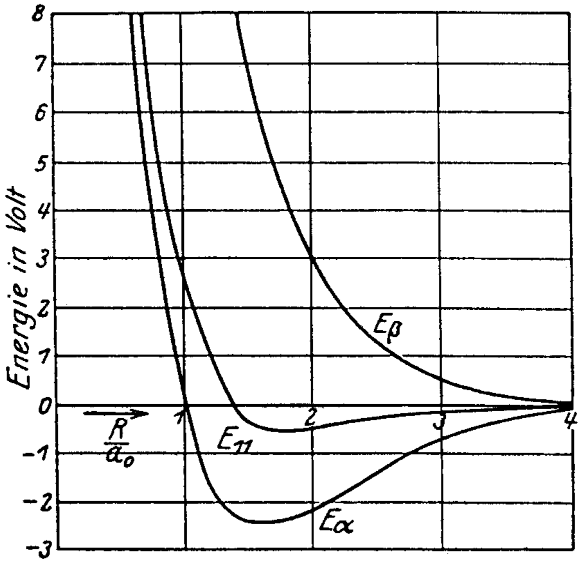
$$\hat{H}^{H_2}_{elec} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + \frac{(-1)(-1)}{r_{12}} + \frac{(+1)(-1)}{r_{1a}} + \frac{(+1)(-1)}{r_{1b}} + \frac{(+1)(-1)}{r_{2a}} + \frac{(+1)(-1)}{r_{2b}}$$

$$\hat{H}^{\bar{H}_2}_{positronic} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + \frac{(+1)(+1)}{r_{12}} + \frac{(-1)(+1)}{r_{1a}} + \frac{(-1)(+1)}{r_{1b}} + \frac{(-1)(+1)}{r_{2a}} + \frac{(-1)(+1)}{r_{2b}}$$

$$|e| = m_e = \hbar = 1$$

$$U^{H_2}_{eff}\left(R_{ab}\right) = \frac{(+1)(+1)}{R_{ab}} + E^{H_2}_{elec}\left(R_{ab}\right)$$

$$U^{\bar{H}_2}_{eff}\left(R_{ab}\right) = \frac{(-1)(-1)}{R_{ab}} + E^{\bar{H}_2}_{positronic}\left(R_{ab}\right)$$



Antichemistry is boring...

Z. Phys. 44, 455 (1927), Hinne Hettema, Quantum chemistry: Classic scientific papers, World Scientific, 2000.

Timeline of some discoveries on Positron and positronium binding to atoms

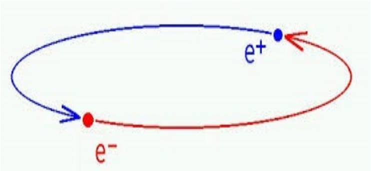
1951: Deutsch produced Positronium (Ps) atom,a bound state of an electron and a positron, it has 10^{-9} seconds lifetime in its singlet ground state and decays spontaneously to gamma photons upon pair annihilation, it was postulated to exist in1934

1951: Ore demonstrated computationally that PsH is a stable species in regard to dissociation to H+Ps and other dissociation channels

1992: PsH, as combination of positronium and hydrogen atoms, was discovered by Schrader and coworkers and its binding energy was measured

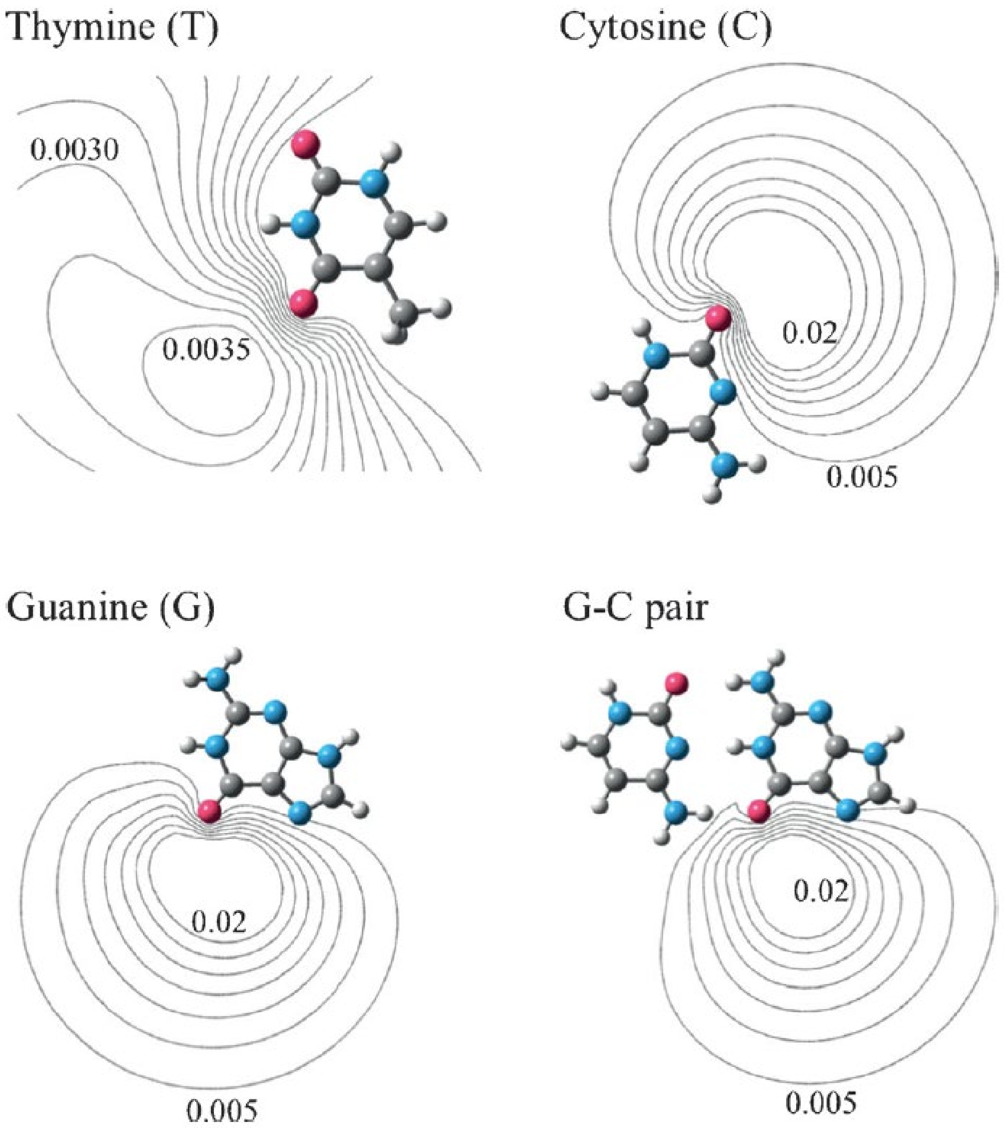
1997: for the first time it was demonstrated by Ryzhikh and Mitroy that a neutral atom, Li, may bind to positron forming e^+Li species

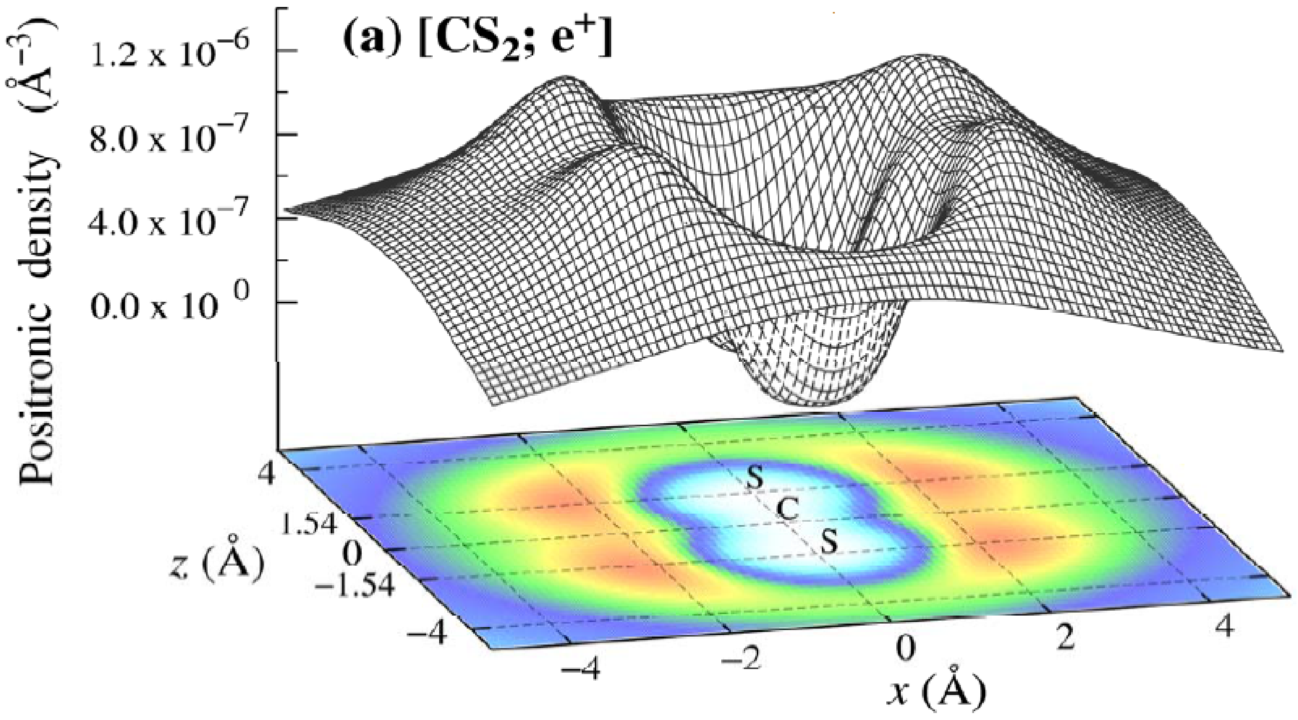
1998-2002: a large number of neutral atoms were demonstrated computaionally to form stable e^+A species A = Be, Na, Mg, Ca, Sr, Cu, Zn, Ag, Cd,.. and simialary stable PsA species, A=Li, Na, K, C, O, ...



JPB 35, R81 (2002), Riv. Nuovo Cimento. 34, 151 (2011), PRL 79, 4124 (1997)

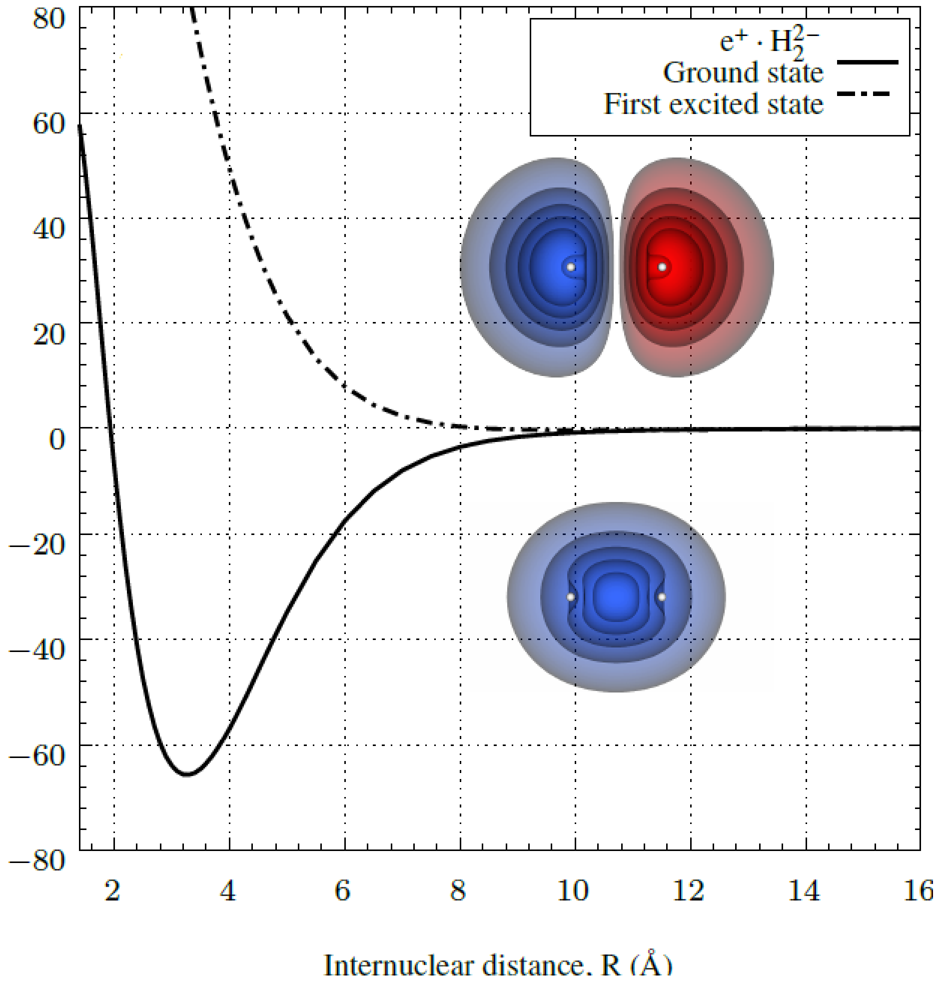
Usual mode of positron and positronium binding to molecules

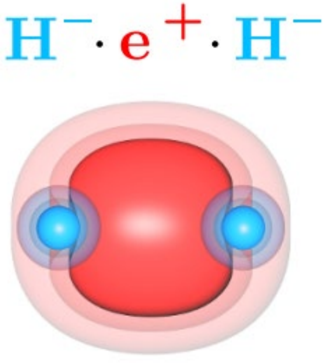




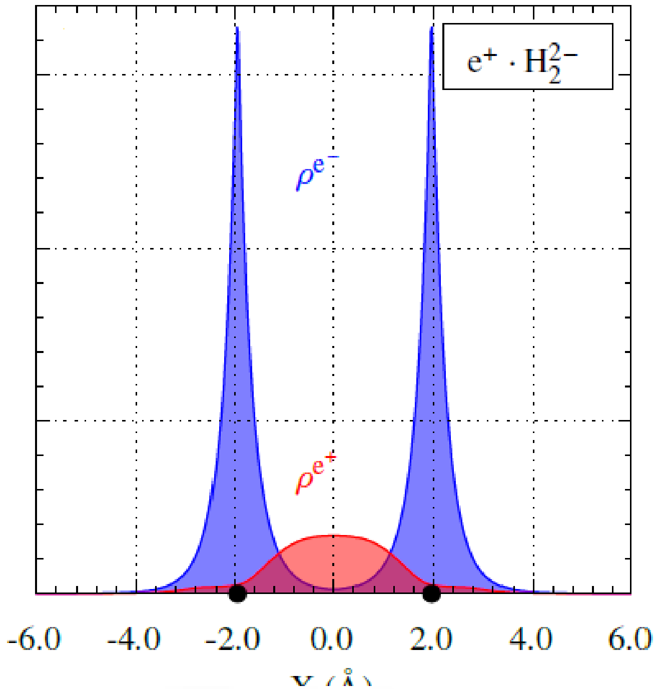
RMP 82, 2557 (2010), JPB 38, R57 (2005), CPC 14, 3458 (2013), PCCP 15, 16208 (2013)

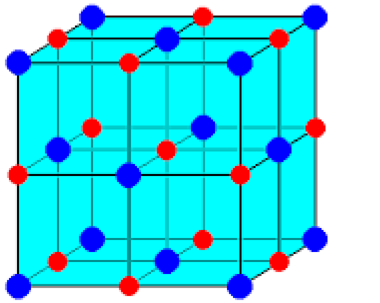
Positron as a bonding agent: Gluonic bonds





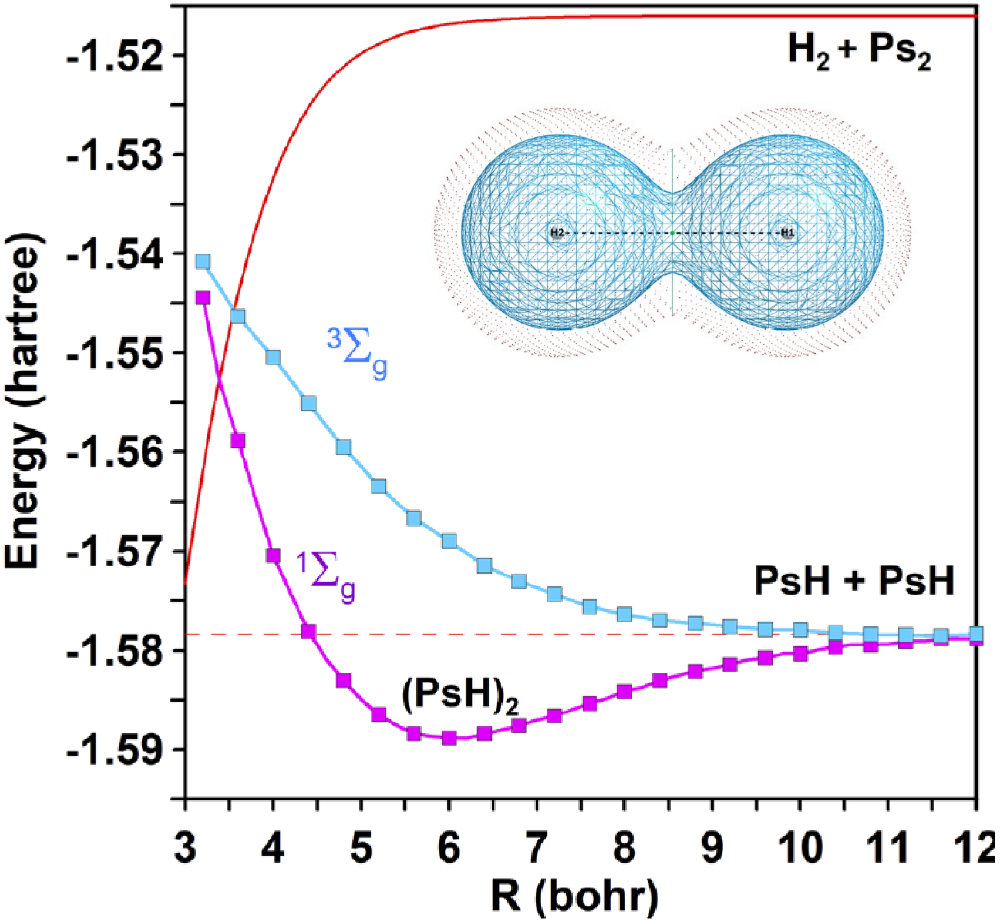
Positron acts as a virtual cation...

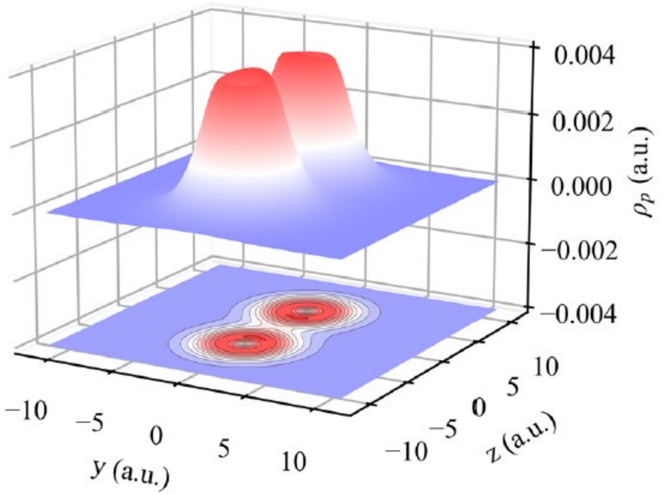


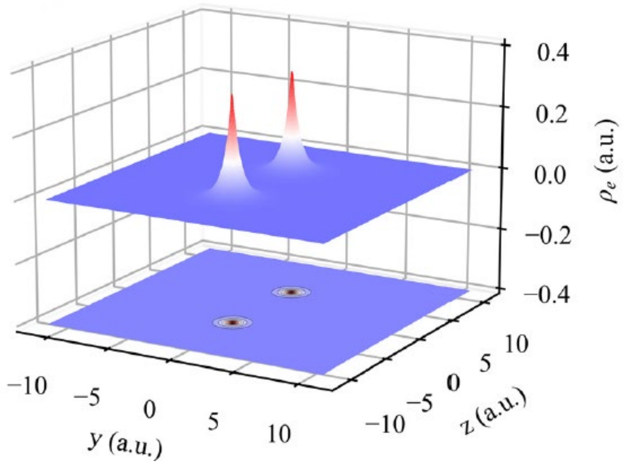


Angew. Chem. Int. Ed. 57, 8859 (2018), CPC 20, 831 (2019), Ashcroft and Mermin, Solid State Physics (1976)

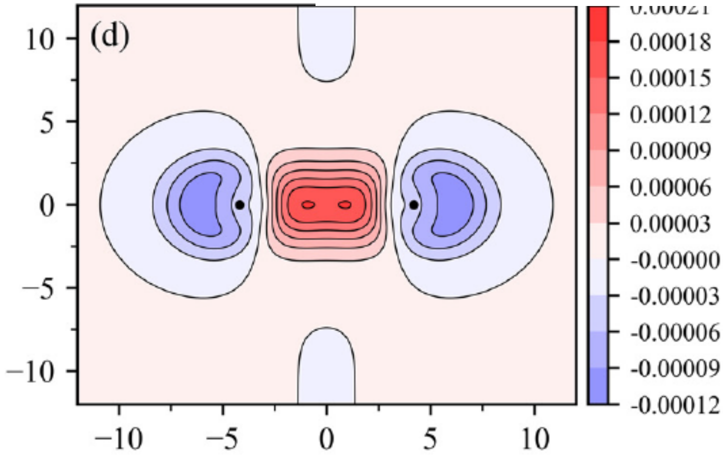
Two positron bonds: The interaction energy and the one-electron/positron densities

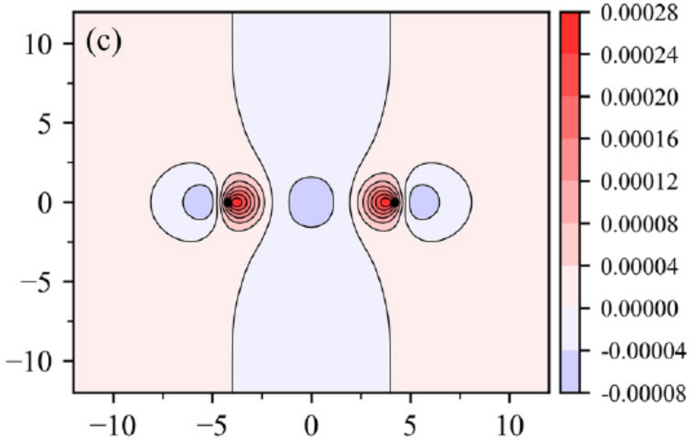






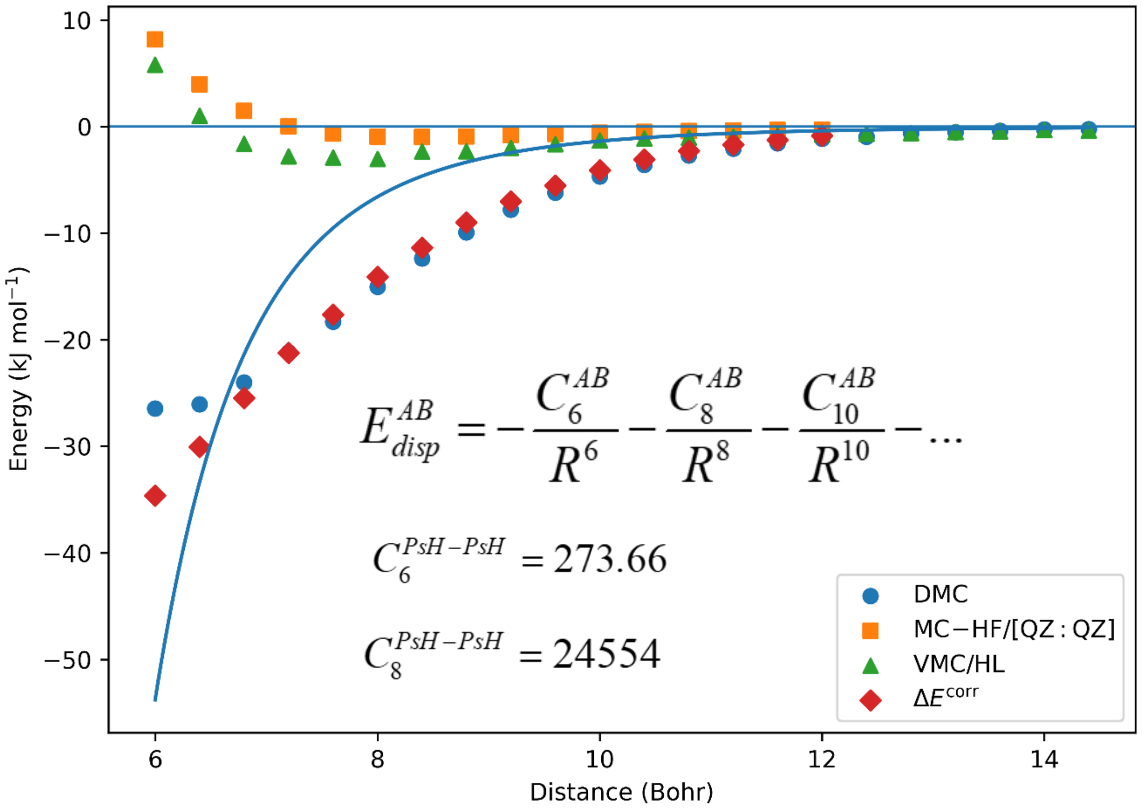
$$\Delta\rho_{\mathrm{p}}(\vec{r}) = \rho_{\mathrm{p}}^{\mathrm{mol.}}(\vec{r}) - \sum_{i}^{P} \rho_{\mathrm{p}}^{\mathrm{atom},i}(\vec{r}).$$

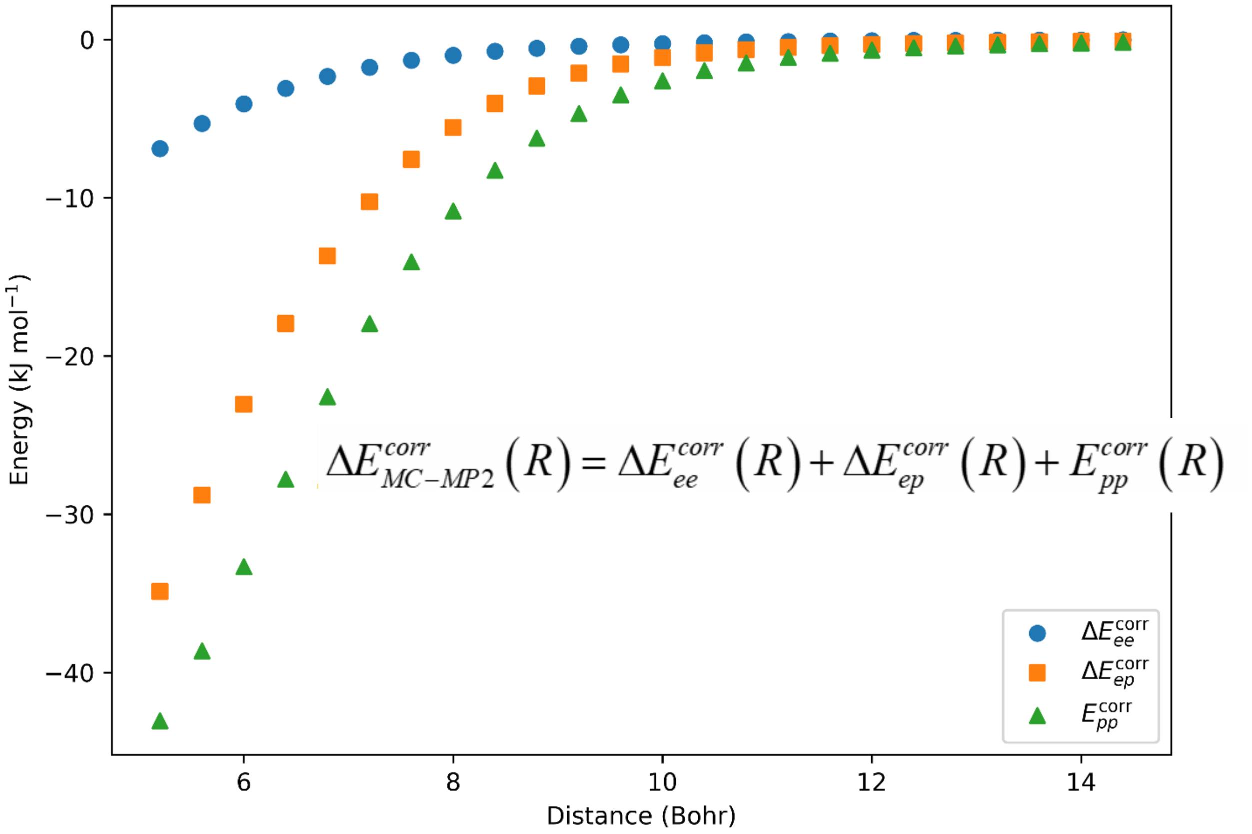




JCP 155, 054306 (2021), PCCP 25, 29531 (2023)

Two positron bonds: Evidence for a "super" van der Waals bond





$$\Psi_{(PsH)_2}^{HL}(1,2) = \frac{1}{\sqrt{2\left(1+S_{AB}^2\right)}}\left(\psi_{PsH}^{A}(1)\psi_{PsH}^{B}(2) + \psi_{PsH}^{A}(2)\psi_{PsH}^{B}(1)\right)$$

$$He-He: D \sim 10^{-3}\,eV$$

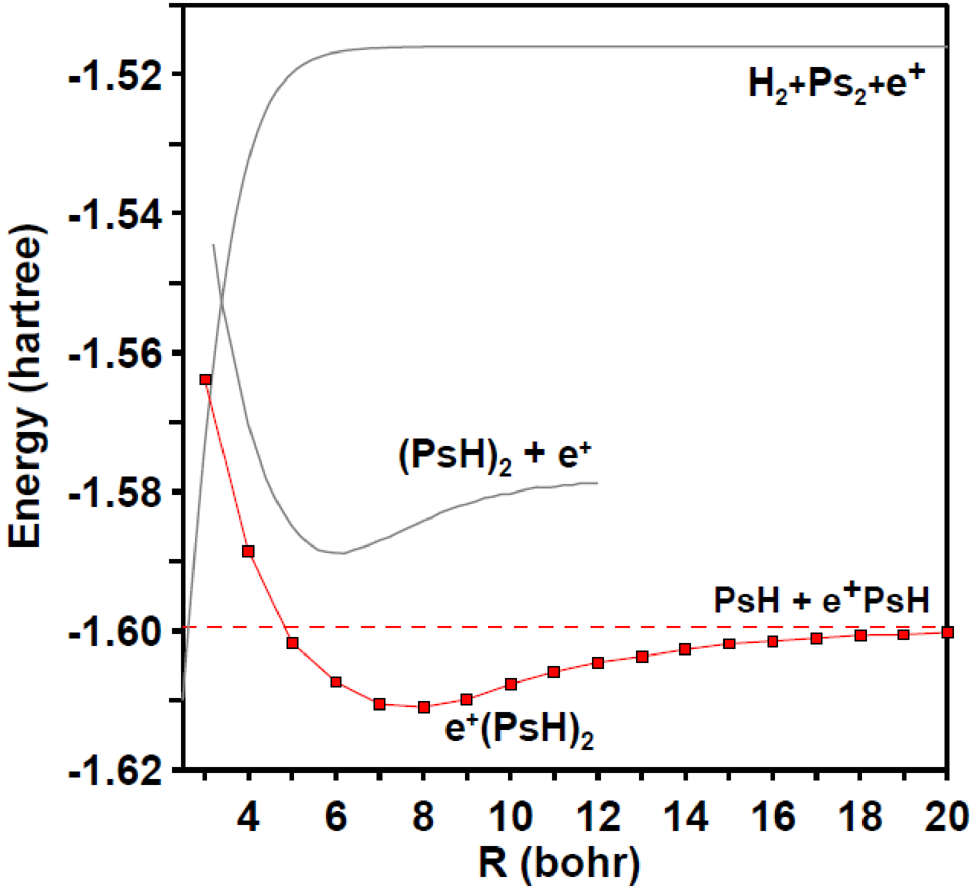
$$Be-Be: D \sim 0.1\,eV$$

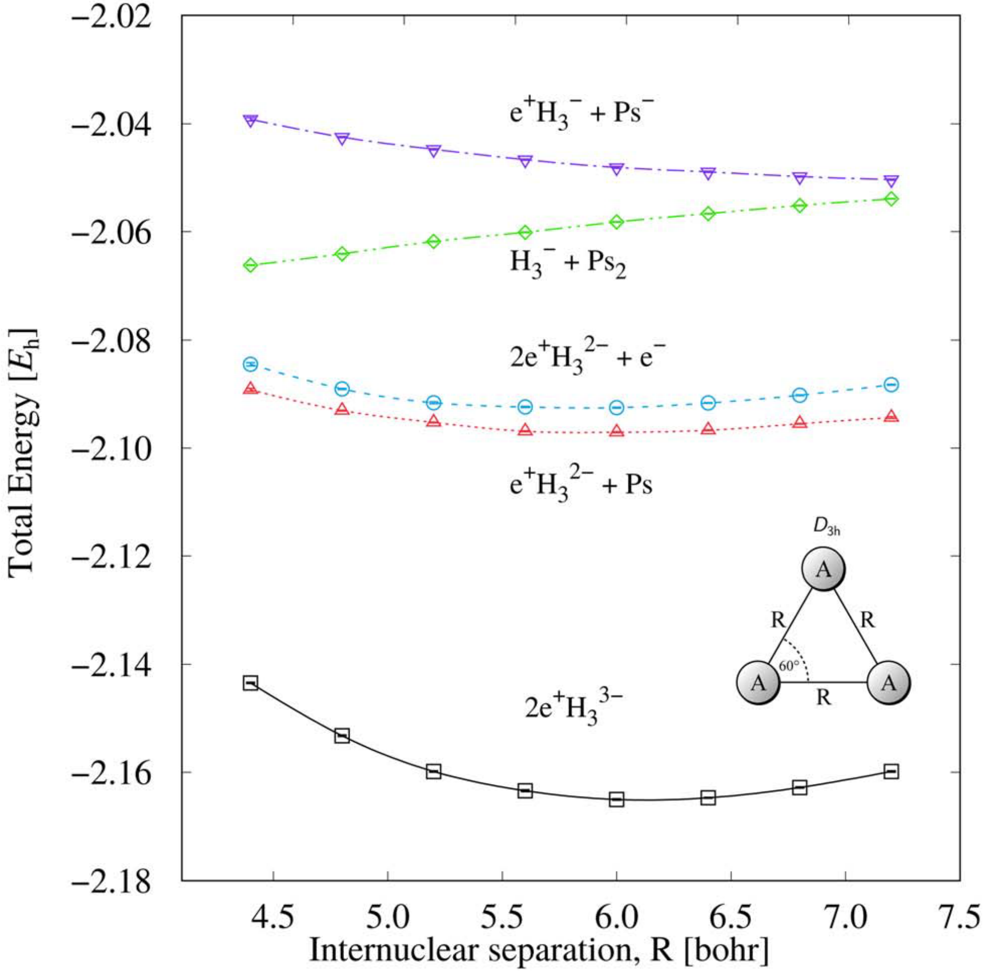
$$PsH-PsH: D \sim 0.3\,eV$$

PCCP 10.1039/d6cp00453a (2026)

Future plans

- What is the nature of three-positron bonds and the three-center two-positron bonds? Is there a universal model, similar to Heitler-London's, for the gluonic bonds?





JCP 155, 054306 (2021), Chem. Sci. 13, 13795 (2022)

Acknowledgments

- Mohammad Goli

- Dario Bressanini

More technical slides…

The multi-component quantum chemistry of positronic species

$$\hat{H}_{elec-pos} = -\sum_{k}^{2}\sum_{i}^{N_k}\frac{\nabla_{i,k}^{2}}{2} - \sum_{k}^{2}\sum_{l>k}^{2}\sum_{i}^{N_k}\sum_{j}^{N_k}\frac{1}{\left|\vec{r}_{i,k}-\vec{r}_{j,l}\right|} + \sum_{k}^{2}\sum_{i}^{N_k}\sum_{j>i}^{N_k}\frac{1}{\left|\vec{r}_{i,k}-\vec{r}_{j,k}\right|} + \hat{V}_{ext}\left(\left\{\vec{R}_\alpha\right\}\right)$$

$$\hat{V}_{ext}\left(\left\{\vec{R}_\alpha\right\}\right) = -\sum_{\alpha}^{M}\sum_{i}^{N_1}\frac{Z_\alpha}{\left|\vec{r}_{i,1}-\vec{R}_\alpha\right|} + \sum_{\alpha}^{M}\sum_{j}^{N_2}\frac{Z_\alpha}{\left|\vec{r}_{j,2}-\vec{R}_\alpha\right|}$$

1=electron, 2=positron

$$\hat{H}_{elec-pos}\Psi_{elec-pos}\left(\left\{\vec{r}_{i,k},\sigma_{i,k}\right\};\left\{\vec{R}_\alpha\right\}\right) = E_{elec-pos}\left(\left\{\vec{R}_\alpha\right\}\right)\Psi_{elec-pos}\left(\left\{\vec{r}_{i,k},\sigma_{i,k}\right\};\left\{\vec{R}_\alpha\right\}\right)$$

How to solve this equation?

$$E_{best} = \underset{Min}{E}\left[\Psi\right]$$

$$\Psi_{trial}\left(\vec{r}_{12,1},\vec{r}_{23,1},\ldots\right) = \sum_{\{i\}}^{\infty} c_{\{i\}}\prod_{k}^{M}\hat{A}_k\psi\left(r_{12,1},r_{23,1},\ldots;\{d\}\right)$$

$$\Psi_{MCHF}\left(\vec{x}_{11},\vec{x}_{21},\ldots,\right) = \left(\frac{1}{\sqrt{N_1!N_2!}}\right)(\det)\left|\phi_{1,1}\left(\vec{x}_{1,1}\right)\phi_{2,1}\left(\vec{x}_{2,k}\right)\ldots\phi_{N_1,1}\left(\vec{x}_{N_1,1}\right)\right|(\det)\left|\phi_{1,2}\left(\vec{x}_{1,2}\right)\phi_{2,2}\left(\vec{x}_{2,2}\right)\ldots\phi_{N_2,2}\left(\vec{x}_{N_2,2}\right)\right|$$

RMP 85, 693 (2013), CR 113, 36 (2013), CR 120, 4222 (2020)

The Quantum Monte Carlo as definite proof for the positron binding capacity

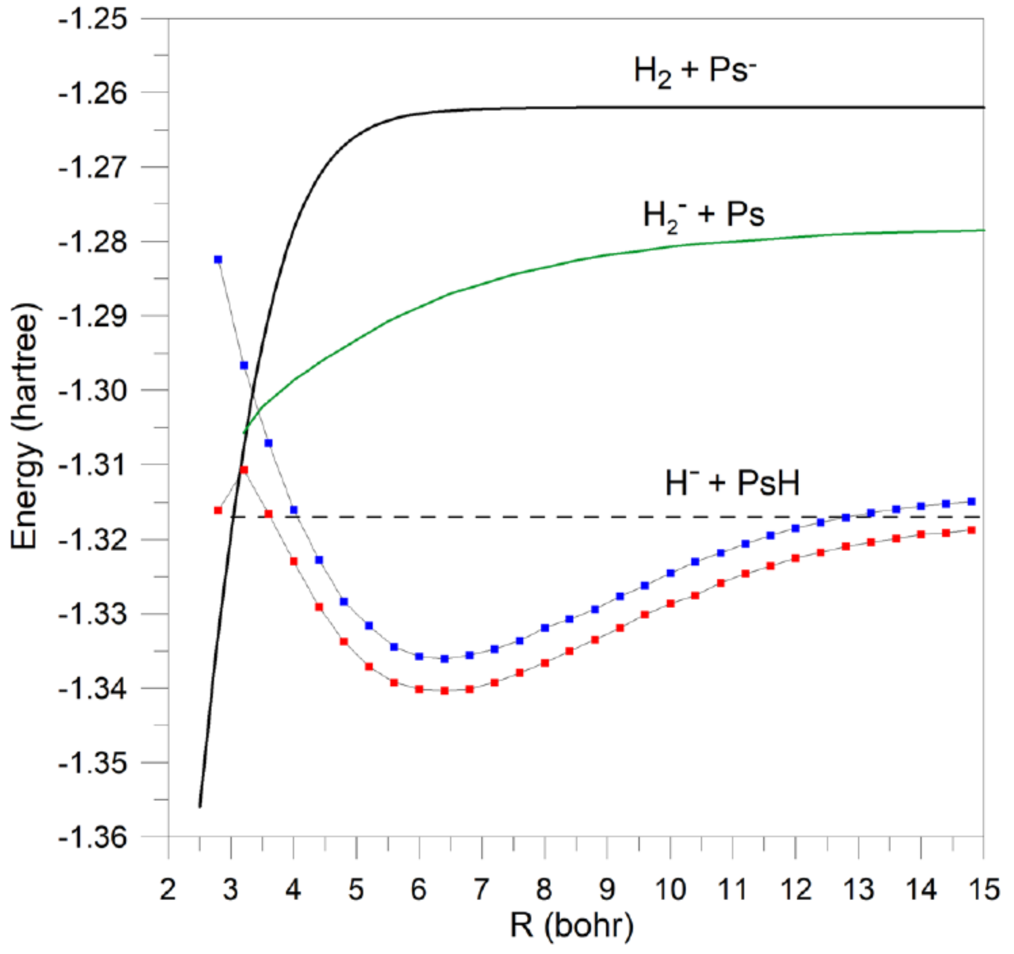


FIG. 1. VMC (blue) and DMC (red) energies for the $e^+H_2^{2-}$ system, together with the energy thresholds for the various dissociation channels as a function of R. The error bars of the individual points are smaller than the size of the symbols.

$$\Psi = \hat{A}\left(1+\hat{i}\right)\prod_{i=1}^{5} f_{iA}(r_{iA}) f_{iB}(r_{iB}) \prod_{i<j} g_{ij}(r_{ij}).$$

$$f_{iX}(r) = g_{ij}(r) = P_3(r) = e^{\frac{ar+br^2}{1+cr}}$$

TABLE I. Total energies (*E*) and binding energies (BE) at the minimum of the PEC calculated by different methods.

Method	R (bohrs)	BE (mhartree)	*E* (hartree)
FCI[a]	6.16	25.1	−1.310 227
CISDTQ[a]	6.16	25.1	−1.318 601
CBS[a]	6.16	29.8	−1.346 256
MC_VMC[b]	6.16	15.8(3)	−1.315 5(2)
MC_DMC[b]	6.16	22.6(1)	−1.339 6(1)
VMC[c]	6.4 ± 0.4	22.7(1)	−1.336 1(1)
DMC[c]	6.4 ± 0.4	23.5(1)	−1.340 4(1)

JCP 154, 224306 (2021)

The nature of the one-positron bond: energy partitioning

$$E_{\text{total}} = \sum_{i}^{P} E_{\text{intra}}(\Omega_i) + \sum_{i}^{P}\sum_{j>i}^{P} E_{\text{inter}}(\Omega_i, \Omega_j)$$

$$= \sum_{i}^{P} \left[T_{\text{e}}(\Omega_i) + T_{\text{q}}(\Omega_i) + V_{\text{e-nuc}}(\Omega_i) + V_{\text{q-nuc}}(\Omega_i) + V_{\text{ee}}(\Omega_i) + V_{\text{qq}}(\Omega_i) + V_{\text{eq}}(\Omega_i)\right]$$

$$+ \sum_{i}^{P}\sum_{j>i}^{P} \left[\begin{array}{l} V_{\text{e-nuc}}(\Omega_i, \Omega_j) + V_{\text{e-nuc}}(\Omega_j, \Omega_i) + V_{\text{q-nuc}}(\Omega_i, \Omega_j) + V_{\text{q-nuc}}(\Omega_j, \Omega_i) \\ + V_{\text{ee}}^{\text{cl}}(\Omega_i, \Omega_j) + V_{\text{ee}}^{\text{xc}}(\Omega_i, \Omega_j) + V_{\text{qq}}^{\text{cl}}(\Omega_i, \Omega_j) + V_{\text{qq}}^{\text{xc}}(\Omega_i, \Omega_j) + V_{\text{eq}}^{\text{cl}}(\Omega_i, \Omega_j) \\ + V_{\text{eq}}^{\text{c}}(\Omega_i, \Omega_j) + V_{\text{eq}}^{\text{cl}}(\Omega_j, \Omega_i) + V_{\text{eq}}^{\text{c}}(\Omega_j, \Omega_i) + V_{\text{nuc-nuc}}(\Omega_i, \Omega_j) \end{array}\right]$$

$$V_{\text{eq}}^{\text{cl}}(\Omega_j, \Omega_i) = -q\int_{\Omega_j} \mathrm{d}\vec{r}_{\text{e}} \int_{\Omega_i} \mathrm{d}\vec{r}_{\text{q}} \frac{\rho_{\text{e}}(\vec{r}_{\text{e}})\rho_{\text{q}}(\vec{r}_{\text{q}})}{|\vec{r}_{\text{e}} - \vec{r}_{\text{q}}|},$$

One-positron bonds have only an exotic electrostatic nature

CPC 20, 831 (2019), PCCP 25, 29531 (2023)

The nature of the two-positron bond: energy partitioning

$$E_{\text{total}} = \sum_{i}^{P} E_{\text{intra}}(\Omega_i) + \sum_{i}^{P}\sum_{j>i}^{P} E_{\text{inter}}(\Omega_i, \Omega_j)$$

$$= \sum_{i}^{P} \left[T_{\text{e}}(\Omega_i) + T_{\text{q}}(\Omega_i) + V_{\text{e-nuc}}(\Omega_i) + V_{\text{q-nuc}}(\Omega_i) + V_{\text{ee}}(\Omega_i) + V_{\text{qq}}(\Omega_i) + V_{\text{eq}}(\Omega_i)\right]$$

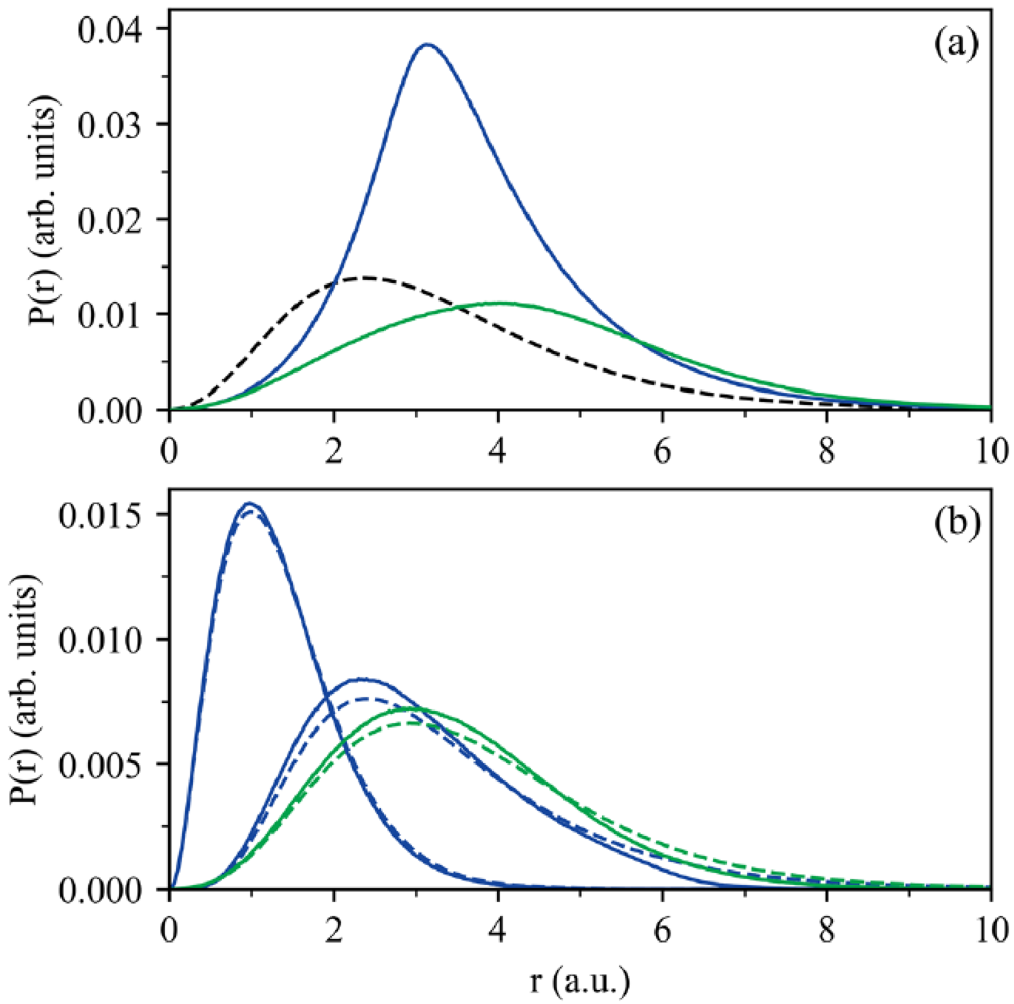
$$+ \sum_{i}^{P}\sum_{j>i}^{P} \begin{bmatrix} V_{\text{e-nuc}}(\Omega_i, \Omega_j) + V_{\text{e-nuc}}(\Omega_j, \Omega_i) + V_{\text{q-nuc}}(\Omega_i, \Omega_j) + V_{\text{q-nuc}}(\Omega_j, \Omega_i) \\ + V_{\text{ee}}^{\text{cl}}(\Omega_i, \Omega_j) + V_{\text{ee}}^{\text{xc}}(\Omega_i, \Omega_j) + V_{\text{qq}}^{\text{cl}}(\Omega_i, \Omega_j) + V_{\text{qq}}^{\text{xc}}(\Omega_i, \Omega_j) + V_{\text{eq}}^{\text{cl}}(\Omega_i, \Omega_j) \\ + V_{\text{eq}}^{\text{c}}(\Omega_i, \Omega_j) + V_{\text{eq}}^{\text{cl}}(\Omega_j, \Omega_i) + V_{\text{eq}}^{\text{c}}(\Omega_j, \Omega_i) + V_{\text{nuc-nuc}}(\Omega_i, \Omega_j) \end{bmatrix}$$

$$V_{\text{eq}}^{\text{c}}(\Omega_i, \Omega_j) = -q \int_{\Omega_i} d\vec{r}_{\text{e}} \int_{\Omega_j} d\vec{r}_{\text{q}} \frac{\rho_{\text{eq}}^{\text{c}}(\vec{r}_{\text{e}}, \vec{r}_{\text{q}})}{|\vec{r}_{\text{e}} - \vec{r}_{\text{q}}|}, \qquad V_{\text{qq}}^{\text{xc}}(\Omega_i, \Omega_j) = q^2 \int_{\Omega_i} d\vec{r}_1 \int_{\Omega_j} d\vec{r}_2 \frac{\rho_{\text{q}}^{\text{xc}}(\vec{r}_1, \vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|},$$

Two-positron bonds have a dual nature, an electrostatic part and a part coming from pure quantum correlations between electrons and positrons

CPC 20, 831 (2019), PCCP 25, 29531 (2023)

The radial distribution functions



(a) Electronic (blue) and positronic (green) radial pair distribution functions depicted with respect to the middle of the inter-proton axis in $(PsH)_2$ (the clamped proton is located at 3 bohr) compared to the same distributions in Ps_2, which are depicted with respect to its center of mass (dashed black). (b) The separate-electron (blue) and separate-positron (green) radial pair distribution functions of PsH (dashed curves) and $(PsH)_2$ (solid curves) with respect to a proton in each species (the proton used as the reference in $(PsH)_2$ is that placed in the left-hand side of the middle of the inter-proton axis). Only the two closest electrons and the closest positron are plotted for $(PsH)_2$.

PCCP 25, 29531 (2023)