Nuclear Fusion Driven by Coulomb Explosion of Molecular Clusters

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No experimental result should be accepted before being confirmed by theory
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The sun produces vast amounts of solar energy necessary to support life on earth by the fusion of hydrogen nuclei, Reaction (1), where H^+, D^+ ($^2H^+$), e^+ and ν denote protons, deuterons, positrons and electron neutrinons, respectively.[1] The nuclear kinetic energy produced per Reaction (1) is $E_{KIN} =$ 0.42 MeV (1 MeV $= 1.6 \times 10^{-13}$ J). As compared to exothermic chemical reactions (with an energy production of 1–5 eV per reaction), such as burning hydrogen, the energy release of nuclear fusion reactions exceeds that of a chemical process by a huge numerical factor of a million.

$$H^+ + H^+ \rightarrow D^+ + e^+ + \nu + E_{KIN} \quad (1)$$

For many years scientists and engineers strived to produce and explore nuclear fusion reactions in the laboratory in an attempt to realize the elusive dream of fusion energy sources. The relevant elementary nuclear reaction for future technological implications involve deuteron–deuteron (dd; $D^+ - D^+$) and deuteron–tritium ($^3H^+$) (dt; $D^+ - T^+$) fusion, Reactions (2) and(3).

$$D^+ + D^+ \rightarrow \begin{cases} ^3He^{2+} + n + 3.27\,\text{MeV} \\ T^+ + H^+ + 4.03\,\text{MeV} \end{cases} \quad (2)$$

$$D^+ + D^+ \rightarrow {}^4He^{2+} + n + 17.6\,\text{MeV} \quad (3)$$

These "big-science" studies attempted to induce fusion in matter under extreme conditions, such as prevailing in the center of the sun, namely high temperatures (10^7 K), pressures and densities. These extreme conditions can be achieved, in principle, in large magnetic and laser implosion devices. A table-top version of such nuclear reaction was recently considered in the controversial Oak Ridge report[2] on a nuclear reactions during acoustic cavitation in deuterated liquids, which constitutes an attempt to provide very high temperatures (10^6 K) and the necessary densities for dd fusion. Further experimental and theoretical work on the validity of the acoustic cavitation "hot fusion" mechanism is called for.

Can Nuclear Fusion be Induced by Chemical Reactions?

The unsuccessful quest for nuclear fusion driven by bulk or surface chemical reactions, for example catalytic dissociation or electrochemical production of hydrogen or deuterium confined in noble metals such as palladium, has a long history. In 1926 the German physicist Fritz Paneth[3] reported the apparent observation of helium from hydrogen absorbed in powdered palladium, which might have originated from Reactions (1) and (2). However, this phenomenon reflected the release of helium impurity from the system rather than on nuclear fusion.[4] In 1935, Adalbert Farkas and Ladislaus Farkas, the founders of physical chemistry in Israel, worked on ortho- and parahydrogen[+] and deuterium chemistry in the Department of Colloid Science at Cambridge University. When passing deuterium gas through a palladium tube they seemed to observe traces of helium, which might have provided evidence for dd nuclear fusion, Reaction (2). However, a search for neutron emission in this system, conducted by Lord Rutherford at the request of the Farkas brothers, was negative and eliminated any possibility for nuclear fusion. In this category of negative results for nuclear fusion belongs the so-called "cold fusion" controversy, which hit the headlines (unfortunately, not only of scientific journals!) in 1989, and did not provide any acceptable scientific information.[5] These spectacular failures are not surprising, as, to the best of our knowledge, no theoretical evidence is available to support any valid mechanism of nuclear fusion driven by chemical reactions in infinite bulk or surface systems.

[+] *Diatomic hydrogen has two forms: orthohydrogen, in which the nuclear spins are parallel, and parahydrogen, in which they are antiparallel. At normal temperatures the gas is 25% parahydrogen; as a liquid it is 99.8% parahydrogen.*

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The failure of the realization of nuclear fusion driven by conventional chemical reaction reflects on "ordinary" molecular systems. Intramolecular nuclear dynamics of "exotic" small molecules provides a valid mechanism for "cold" fusion. These "exotic" molecules involve the replacement of electrons by negative muons μ (whose mass is 207-fold the electron mass). When a heavy negative muon replaces an electron in the H_2 (or D_2) molecule, a dramatically enhanced screening of the H^+-H^- (or D^+-D^- repulsion in the exotic $H^+H^+e\mu$ (or $D^+D^+e\mu$) diatomic molecule occurs. This screening effect enables the close approach of the $H^+ + H^+$ or $D^+ + D^+$ pair to promote pp or dd nuclear fusion via tunneling in the exotic molecule. This "cold" fusion process was predicted by Andrei D. Sakharov in 1940 and experimentally observed by Louis Alvarez in 1956.[6] The low yield of this process is limited by the short lifetime (microseconds) of the muon and by its reaction with the He products. This legitimate muon-catalyzed fusion mechanism, for which unambiguous experimental evidence exists and which is supported by theory, is only of methodological interest.

Nuclear Fusion Driven by Cluster Dynamics

An alternative avenue for the induction of nuclear fusion reactions involves the utilization of the ultrafast, high-energy dynamics of multicharged large finite chemical systems, namely charged molecular clusters such as $(D_2)_n^{Z+}$, $(D_2O)_n^{Z+}$ or $(CD_4)_n^{Z+}$, for the realization of sufficiently high nuclear energies, in the energy domain of nuclear physics. The search for nuclear fusion driven by cluster dynamics started with the 1989 Brookhaven experiments[7] on the high-energy collisions of deuterated charged clusters, driven in a particle accelerator, with a deuterated target. Unfortunately, the initial positive experimental results for dd fusion (which were in contrast with molecular dynamics simulations) were not properly interpreted.[7] While neutron emission was documented, these experiments were fraught with inadequate mass resolution, so that nuclear fusion originated from the well-known (and uninteresting) D^+-deuterated wall collisions and did not provide information on cluster impact fusion.

During the last two years, compelling experimental[8, 9] and theoretical[10–12] evidence was advanced for nuclear fusion driven by Coulomb explosion (NFDCE) of an assembly of deuterium-containing clusters (Figures 1 and 2). Highly charged molecular clusters can be prepared by the irradiation of a cluster beam by ultrashort (tens of femtoseconds) and ultraintense ($I = 10^{15}$–10^{19} W cm^{-2}) laser pulses (Figure 1). Femtosecond electron dynamics in clusters, involving inner ionization on a time scale of 1–5 fs and outer ionization on a time scale of 5–20 fs, results in multielectron ionization. For the intensity domain of $I = 10^{16}$–10^{17} W cm^{-2} the cluster molecules lose all their valence electrons, while for the highest intensity range of $I = 10^{18}$–10^{19} W cm^{-2} inner shell and valence electrons can be stripped off.[11] The Coulomb instability of the highly charged finite cluster triggers simultaneous and concurrent ultrafast Coulomb explosion on the time scales of 10–100 fs (Figure 3). Ultrahigh ion energies in the energy range of 1 keV–1 MeV are released by cluster Coulomb explosion. In an assembly of deuterium- or tritium-containing exploding charged clusters, the collisions of the high-energy d or t nuclei in the 1–10 keV domain (Figure 4) originating from different clusters may induce dd or dt nuclear fusion, Reaction (2) or (3), in the chemical physics laboratory (Figure 2). The dd fusion, Reaction (2), driven by Coulomb explosion of totally ionized $(D_2)_n$ clusters (cluster radius $R_0 = 10$–50 Å and number of constituents $n = 400$–20000) in an intense laser field ($I \sim 5 \times 10^{17}$ W cm^{-2}) was experimentally

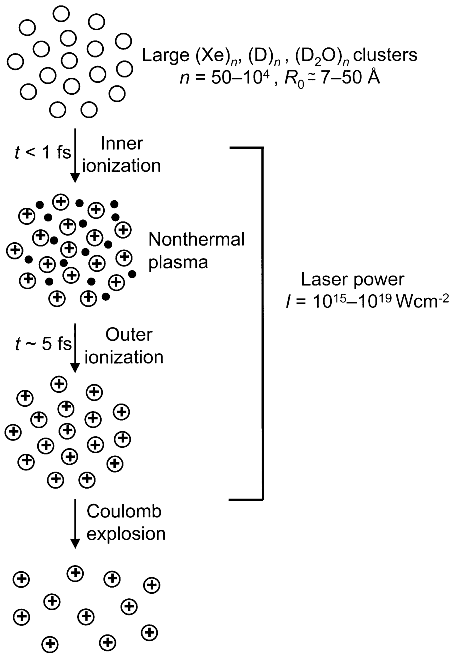

Figure 1. An artist's view on ultrafast electron and ion dynamics for molecular clusters in intense laser radiation fields.

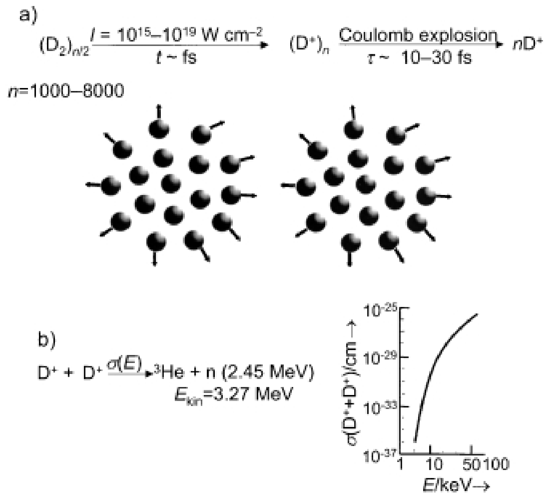

Figure 2. a) Nuclear fusion driven by Coulomb explosion of deuterium clusters. Multielectron ionization in an ultrahigh laser field strips, via consecutive inner and outer ionization, the $(D_2)_{n/2} \equiv (D)_n$ clusters of all their electrons. Parallel, and concurrent with the outer ionization process, cluster Coulomb explosion occurs. For clusters in the size domain n = 1000–8000 the deuterons' maximal energies are in the range $E_M = 1$–3 keV. b) Energetic deuterons ($^2H^+$, D^+) emerging from different clusters in the beam undergo dd nuclear fusion, whose energy-dependent cross-section σ is shown.

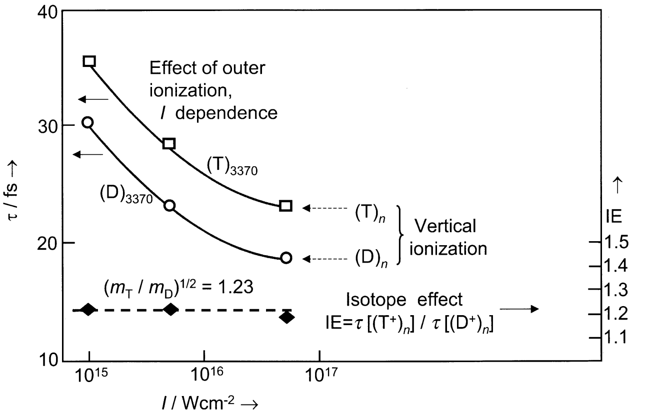

Figure 3. *The time-resolved dynamics of the Coulomb explosion of large $(D_2)_{n/2}$ and $(T_2)_{n/2}$ clusters (n = 3370) in intense laser fields (I = 10^{15} – 10^{17} W cm^{-2}). The Coulomb explosion lifetimes τ (characterizing the time for the doubling of the cluster initial size) were obtained from molecular dynamics simulations for femtosecond electron and nuclear dynamics using attosecond time steps (refs. [11] and [12]). The enhancement of the outer ionization in higher laser fields shortens τ. The Coulomb explosion lifetimes for initially totally ionized clusters (prepared by vertical ionization) are given by $\tau\,[fs] = 2.137\, q^{-1}\, [m\rho^{-1}]^{1/2}$, where q is the constituent charge in its mass and ρ [Å^{-3}] is the cluster density, being independent of the cluster size, as marked by arrows ← $(T)_n$ and ← $(D)_n$. These lifetimes for vertically ionized clusters represent the τ values well at the highest intensity of I = 10^{17} W cm^{-2}. The isotope effect (IE) on the Coulomb explosion lifetimes is well accounted for by the square root of the mass ratio.*

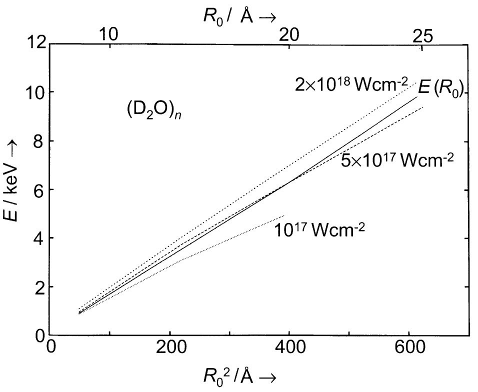

Figure 4. *The cluster size dependence of the maximal kinetic energy of deuterons D^+ from Coulomb explosion of $(D_2O)_n$ clusters, where the cluster radius varies in the range R_0 = 8 – 25 Å (n = 55 – 2170). The dashed lines represent the results of simulations (refs. [11] and [12]) at the indicated laser intensities. The solid line represents the analytic expression for the energy (refs. [10] and [11]) $E(R_0)\,[eV] = (4\pi B/3)(2q_D + q_0)q_D\rho_0 R_0^2$, where $q_D = 1$ and $q_O = 6$, ρ_0 [Å^{-3}] is the density and B = 14.385 eV Å^{-1}. The cluster size dependence of the maximal kinetic energy $E(R_0) \propto R_0^2$ is well obeyed at I = 10^{17} W cm^{-2}.*

observed in the Lawrence Livermore laboratory.[8, 9] The Tel Aviv work[10–12] proposed and demonstrated, by molecular dynamics simulations, that an effective way to produce energetic D^+ or T^+ nuclei for fusion involves multielectron ionization and Coulomb explosion of molecular heteroclusters of deuterium/tritium bound to heavy atoms. Adequate clusters for high-energy Coulomb explosion involve multielectron ionized heavy water clusters $(D^+D^+O^{6+})_n$, $(D^+T^+O^{6+})_n$, or heavy methane clusters $(C^{q+}D_4^+)_n$, $(C^{q+}T_2^+D_2^+)_n$ (with n = 100 – 10^5, R_0 = 10 – 80 Å, and q = 4 or 6), where the heavy multielectron ions (O^{6+}, C^{4+}, or C^{6+}) act as energetic triggers for driving the light D^+ or T^+ ions to considerably higher kinetic energies than for totally ionized homonuclear $(D_2)_n$ or $(DT)_n$ clusters of the same size. For example, the maximal energy E_M of deuterons produced by Coulomb explosion of a homonuclear $(D^+)_{3376}$ cluster (R_0 = 25.4 Å) is E_M = 1.9 keV, while the heteronuclear $(D^+D^+O^{6+})_{2172}$ cluster with the same radius (R_0 = 25 Å) provides deuterons with E_M = 10.8 keV. An extreme way to obtain highly effective energetic triggers to drive deuterons to very high energies can be accomplished by multielectron ionization of mixed $(Xe)_m(D_2)_n$ clusters or of $(DI)_n$ heteroclusters, where heavily charged Xe^{+26} or I^{+26} ions, with huge charges, can be produced in very intense (I = 10^{19} W cm^{-2}) laser fields. In addition, kinematic effects, which manifest a sharp energy maximum of the light-ion kinetic energy spectra emerging from deuterium-containing molecular heteroclusters, provide a supplementary contribution to the efficiency of the NFDCE (Figure 5). The Tel Aviv work determined the cluster size dependence of the fusion reaction yields Y per laser pulse (Figure 6), for example, for the NFDCE of $(D_2O)_n$ and $(DTO)_n$ clusters with R_0 = 30 Å, Y = 10^6 for the dd reaction (Figure 6) and Y = 10^8 for the dt reaction. Thus the feasibility of the NFDCE of deuterium-containing clusters was established.

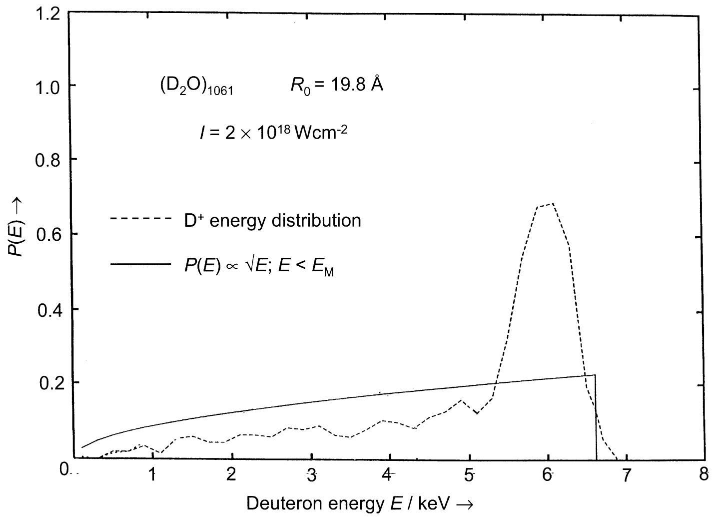

Figure 5. *The kinetic energy distribution P(E) of the D^+ ions for Coulomb explosion of heteronuclear $(D_2O)_{1061}$ clusters subjected to multielectron ionization at I = 10^{18} W cm^{-2}. The dashed line, which represents the simulation results, peaks in the vicinity of the maximal energy E_M = 6.7 keV and exhibits a marked variation from the relation $P(E) \propto (E)^{1/2}$ inferred from the cluster size equation $E(R_0) \propto R_0^2$ (ref. [11]). The peak in P(E) around E_M manifests kinematic effects in the Coulomb explosion of $(D^+D^+O^{+6})_n$ heteroclusters (ref. [11]).*

Perspectives of Nuclear Fusion Driven by Cluster Coulomb Explosion

Of considerable interest are the perspectives of the NFDCE of deuterium- or tritium-containing homonuclear and heteronuclear clusters in the Chemical Physics laboratory for the production of short (100 ps – 10 ns) neutron pulses,[9, 11] which may be instrumental in the exploration of time-resolved structural studies of biomolecules or large molecules. The utilization of NFDCE of deuterium-containing heteronuclear

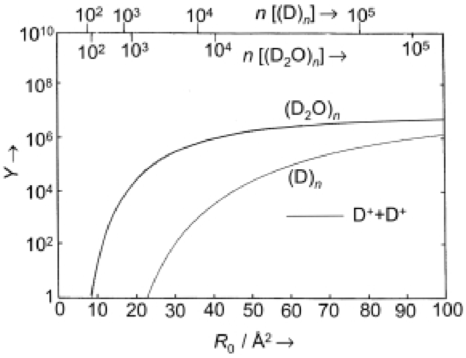

Figure 6. The cluster size dependence of the neutron yields Y *for dd NFDCE per laser pulse (under the experimental conditions of ref. [8]) calculated from molecular dynamics simulations for multielectron ionization and Coulomb explosion of homonuclear* $(D)_n$ *and heteronuclear* $(D_2O)_n$ *clusters* ($n = 10^2 - 10^5$) *in very intense* ($I = 10^{17}$ W cm^{-2}) *laser fields (ref. [11]). The number of atoms corresponding to a cluster radius* R_0 *is shown on the upper scale for the homonuclear and heteronuclear clusters. The NFDCE for the heteronuclear clusters manifests a considerably larger neutron yield than for the homonuclear clusters of the same size, exhibiting energetic and kinematic effects, as discussed in the text.*

clusters will greatly enhance the intensity of the neutron pulse. In addition, some nuclear fusion reactions involving protons and heavy nuclei, such as the $^{12}C^{6+} + H^{+} \rightarrow {}^{13}N^{7+} + \gamma$ reaction, are of astrophysical interest for the carbon–nitrogen–oxygen (CNO) cycle in hot stars. The CNO cycle of nuclear fusion, which supplies energy to the hot stars, is catalyzed by $^{12}C^{6+}$, which is regenerated.[1] The $^{12}C^{6+} + H^{+}$ NFDCE can be induced by multielectron ionization of sufficiently large methane clusters ($R_0 =$ 120 Å), providing information on the cross-sections and dynamics of elemental nuclear processes in astrophysics.

The NFDCE of molecular clusters induced by multielectron ionization and Coulomb explosion involves a "cold–hot" fusion mechanism, where the cluster beam constitutes a cold (or even ultracold) target, while the Coulomb explosion of the assembly of clusters provides the high energy required to induce nuclear fusion. The realization of the NFDCE of molecular clusters constitutes a novel and significant implication of ultrafast electron–nuclear dynamics of large finite systems in ultraintense laser fields.

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