Nuclear Fusion induced by Coulomb Explosion of Heteronuclear Clusters

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We propose a new mechanism for the production of high-energy ($E > 3$ keV) deuterons, suitable to induce dd nuclear fusion, based on multielectron ionization and Coulomb explosion of heteronuclear deuterium containing molecular clusters, e.g., $(D_2O)_n$, in intense (10^{16}–2×10^{18} W/cm^2) laser fields. Cluster size equations for E, in conjunction with molecular dynamics simulations, reveal important advantages of Coulomb explosion of $(D_2O)_n$ heteronuclear clusters, as compared with $(D)_n$ clusters. These involve the considerably increased D^+ kinetic energy and a narrow, high-energy distribution of deuterons.

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Extraordinary facets of ultrafast electronic dynamics (on the time scale of ~1–10 fs) and nuclear dynamics (on the time scale of ~10–100 fs) of large finite systems, e.g., molecular clusters, are triggered by their interaction with ultraintense laser fields (intensity 10^{14}–10^{18} W/cm^{-2}) [1–5]. Femtosecond electron dynamics involving inner and outer cluster high-order multielectron ionization [6,7], which strips the cluster atoms of their valence outer shell electrons, is accompanied by simultaneous and concurrent Coulomb explosion, which is ultrafast on the time scale of intramolecular nuclear motion. Ultrahigh ion energies are released, being in the range of keVs for small molecular clusters (e.g., $Xe_n, n \leq 13$) and 10 keV–1 MeV for larger clusters (e.g., $Xe_n; n > 200$) [6], reaching the energy domain of nuclear physics. Deuterium or tritium clusters are of central interest as their complete multielectron ionization will result in nuclear matter, undergoing Coulomb explosion and providing a high-energy (keV) source of deuterons or tritons.

It was recently reported [5] that Coulomb explosion of large deuterium clusters (average cluster radii $R_0 = 10$–50 Å) subjected to very strong laser fields ($I = 5 \times 10^{17}$ W/cm^{-2}) drives dd fusion. Zweiback *et al.* [5] proposed that the fusion reaction observed by them originates from collisions of deuterons from different clusters. We propose a new mechanism for multielectron ionization and Coulomb explosion of heteronuclear molecular clusters containing deuterium and heavy atoms, providing a source of high-energy (3–10 keV) deuterons with a narrow energetic distribution, which is suitable to induce dd nuclear fusion.

Vertical multielectron ionization of molecular clusters involves the separation of time scales between the removal of all unbound electrons produced by inner ionization and the cluster expansion due to Coulomb explosion. For a homonuclear cluster with identical charges (q in e units) on each atom and uniform atomic density ρ (in Å^{-3}), the kinetic energy E (per ion in eV) is maximal for ions at the cluster surface at the initial cluster radius R_0 (in Å) being given by [8]

$$E(R_0) = (4\pi/3)Bq^2\rho R_0^2, \tag{1}$$

where $B = 14.385$ eV. Equation (1) provides a unique case of a cluster size equation (CSE) [9], with the scaling law $E \propto R_0^2$ constituting an exception for CSEs, which usually converge to the condensed phase ($R_0 \to \infty$) limit [6,9].

Equation (1) implies that the kinetic energy of the product ions increases with the ionic charge q. Accordingly, multielectron atoms, which can be highly ionized, will provide ions of considerably higher kinetic energy (e.g., ~40 keV for Coulomb explosion of Xe_{1000} [6]). In order to produce energetic deuterium (or tritium) ions of one-electron atoms, we propose the utilization of Coulomb explosion of heteronuclear molecular clusters $(D_\ell B_k)_n$ consisting of $D_\ell B_k$ molecules with light one-electron D atoms and heavy multielectron B atoms. The highly charged B^{+q_B} ions will provide a trigger for driving the D^+ ions to high kinetic energies. Typical candidates for clusters whose Coulomb explosion will provide a high-energy ($E > 3.0$ keV) D^+ source may involve D_2 doped Xe clusters, $(DF)_n$ or $(D_2O)_n$.

Two immediate advantages of the use of Coulomb explosion of heteronuclear deuterium containing clusters are (i) a considerable increase in the kinetic energy of the light D^+ ions, and (ii) enhanced radial expansion of the high-energy light ions. To assess the implications of kinetic energy increase [point (i)], we consider the modification of Eq. (1) for a heterocluster with the kinetic energies $E(R_0)$ of the light D^+ ions initially located at the cluster periphery ($R = R_0$), to be given by

$$E(R_0) = (4\pi/3)B(q_D\rho_D + q_B\rho_B)q_D R_0^2, \tag{2}$$

or

$$E(R_0) = Bn(lq_D + kq_B)q_D/R_0, \tag{2'}$$

where $q_D = 1$, $q_B \gg 1$, and ρ_D and ρ_B are the atomic densities of the light D and the heavy B atoms, respectively. Equation (ii) provides a higher kinetic energy than Eq. (1), with the energy increase factor (for $\rho_D \sim \rho_B$) being $\sim 1 + (q_B/q_D)$.

The enhanced radial expansion of the energetic D^+ ions [point (ii)] can be inferred from the dynamics of the Coulomb explosion in the heteronuclear cluster. The accelerations of the light and heavy ions initially located at the same distance R from the cluster center are related by $\eta = q_D m_B / q_B m_D$, where m_B and m_D are the masses (in amu) of the heavy and light atoms, respectively. When the heavy atom is deprived of all its valence electrons, we expect that $\eta > 1$ for all heavy B atoms in the periodic table, including Li. When $\eta > 1$, the light atoms attain a higher velocity than the heavy atoms at the same R, so that a substantial portion of the light ions is expected to move out from the initial configurational framework of the heavy ions. Provided that the cross section for $D^+ + B^{+q_B}$ collisions is sufficiently small [10], the D^+ ions initially located inside the cluster (at $R < R_0$) will over-run the heavy ions, gaining a higher energy than that given by Eq. (2).

We have studied outer ionization and Coulomb explosion of heteronuclear $(D_2O)_n$ clusters and of homonuclear $(D)_n$ clusters by molecular dynamics simulations previously described [6]. The simulations of the ionization process show that the atoms are deprived from their outer shell electrons in a few fs [6]. Accordingly, we do not explicitly treat the inner ionization [11] and consider the initial state of the $(D)_n$ clusters as consisting of n uniformly distributed deuterons and n unbound electrons. The $(D_2O)_n$ cluster is described as uniformly distributed D_2O molecules with the density $\rho = 0.035$ Å^{-3} per molecule. The DO distance is 0.97 Å and the D-O-D angle was taken at 90°. The multielectron ionization of the O atoms is restricted to the valence outer shell electrons. The initial state of the $(D_2O)_n$ cluster consists of O^{6+} ions, $2n$ deuterons, and $8n$ unbound electrons. Since the inner $(1s)^2$ shell of the O atom is very compact, we consider only the Coulomb interaction of the O^{6+} ion with the other charged particles. The Coulomb forces also describe the electron-electron, electron-deuteron, and deuteron-deuteron interactions. The Coulomb potential of the electron-electron interaction is modified by a smoothing term in order to avoid a steep increase in forces at very small distances and the violation of energy conservation [6,11]. The clusters are subjected to the irradiation of a Gaussian-shaped laser pulse shape with a temporal half full width at a half maximum of 25 fs. The frequency is $\nu = 0.35$ fs.

The dependence of the maximal kinetic energy E of the deuterons from Coulomb explosion of $(D)_n$ clusters ($n = 900$–$8000, R_0 = 19.5$–40 Å) on the laser intensity I [$5 \times (10^{14}$–$10^{17})$ W/cm^2] reveals an increase of E with increasing I at lower I followed by saturation at high I (Fig. 1). The I interval, where E begins to decrease markedly with decreasing I, is cluster size dependent and determines the limit of efficient outer ionization. To quantify this limit, we define the saturation intensity I_e, where the energy E makes up for 85% of the energy of the saturation level E_M, i.e., $E(I_e) = 0.85 E_M$. In Fig. 2 we display the saturation energies E_M and the saturation intensities I_e, where we have also included the results for a small $n = 55$ cluster for which $I_e = 11 \times 10^{14}$ W/cm^2, being an order of magnitude higher than the power required for multielectron ionization of the D_2 molecule [12]. Both E_M and I_e follow the quadratic size dependence, being proportional to R_0^2 (Fig. 2). The CSE $E_M \propto R_0^2$ is in accord with the theoretical predictions of Eq. (1).

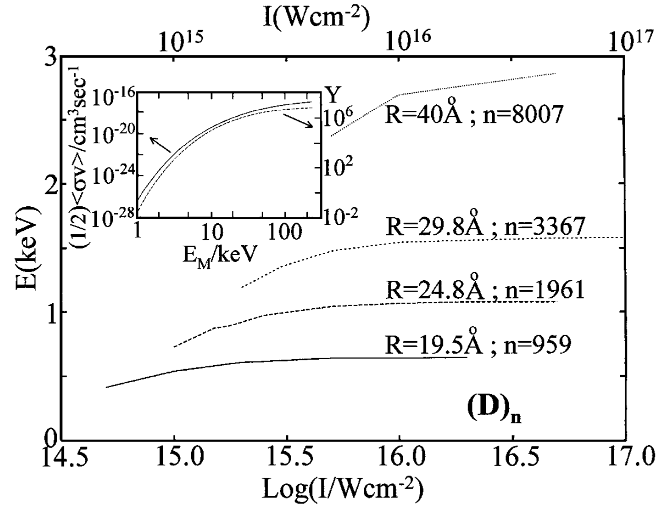

FIG. 1. Simulations of the Coulomb explosion of $(D)_n$ clusters, presenting the dependence of the D^+ maximal energy on the laser intensity. Cluster sizes are marked on the curves. The inset shows the neutron fields Y for the $d + d \rightarrow {}^3\mathrm{He} + n$ reaction, $Y = \frac{1}{2}\langle \sigma v \rangle \rho^2 V \tau$, where $\langle \sigma v \rangle$ is the collision velocity averaged cross section σ [13] with the energy distribution $P(E) = AE; E < E_M$ and $P(E) = 0; E > E_M$ where ρ is the effective density, $V = \pi r^2 \ell$ is the reaction volume, and $\tau = \ell / 6\langle v \rangle$ is the flight time with $\langle v \rangle$ being the average velocity. The geometrical parameters and ρ are taken from Ref. [5].

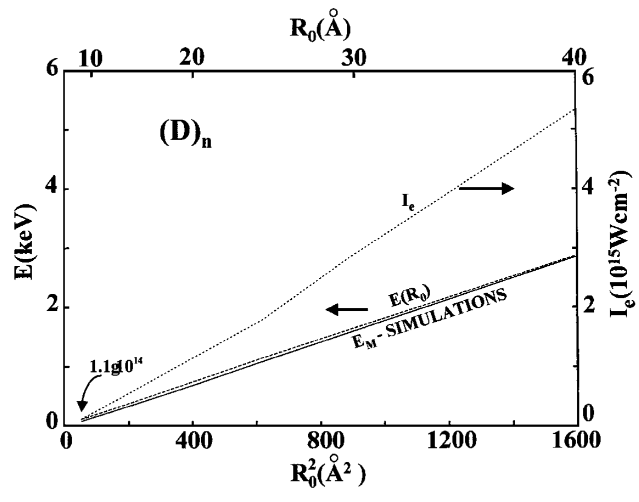

FIG. 2. The cluster size dependence of the D^+ energies at the saturation level (E_M) and the saturation intensities (I_e) from simulations of the Coulomb explosion of $(D)_n$ clusters. Also given is the CSE for $E(R_0)$, Eq. (1).

The fusion parameter $\langle \sigma v \rangle$ was evaluated by using the dd reaction cross section $\sigma(E)$ [13] and by averaging over the collision angle and the colliding particle energies for the deuteron energy distribution in the Coulomb explosion (inset of Fig. 1). The neutron yield Y was calculated for the experimental conditions of Ref. [5]. We found that effective dd fusion will be induced for $E_M \geq 3.0$ keV, i.e., $R_0 \geq 40$ Å, for which $Y \geq 10^2$. The quadratic R_0 dependence of I_e (Fig. 2) implies that for $R_0 = 40$ Å the limit of the laser power is $I_e \simeq 5.5 \times 10^{15}$ W/cm^{-2}. This value of I_e is considerably lower than the laser power $I = 5 \times 10^{17}$ W/cm^2 employed by Zweiback *et al.* [5], confirming the possibility of complete deuterium cluster ionization under these experimental conditions. dd fusion was reported [5] from $(D)_n$ clusters with an average radius $R_0 > 15$ Å, which is smaller than the lower limit $R_0 \geq 40$ Å estimated herein. The dichotomy between experimental data [5] and the present theory requires further elucidation of the size distribution of the cluster radii in the important experiment by Zweiback *et al.* [5].

Simulations for the multielectron outer ionization and Coulomb explosion dynamics of $(D_2O)_n$ ($n = 55-2171$, $R_0 = 7.0-25.0$ Å) clusters (Fig. 3) confirm our predictions for the increased deuteron energy from heteronuclear clusters. Heteronuclear clusters provide considerably higher D^+ kinetic energies than homonuclear clusters of the same size, e.g., for $I = 5 \times 10^{16}$ W/cm^{-1}, both the $(D_2O)_{459}$ heterocluster ($R_0 = 14.85$ Å) and the $(D)_{8007}$ homonuclear cluster ($R_0 \equiv 40$ Å) provide deuterons with $E_M \simeq 2.8$ keV. High-energy D^+ with $E_m = 10.5$ keV are already produced from moderately small $(D_2O)_{2171}$ ($R_0 = 25$ Å) clusters. From the CSE $E_M \propto R_0^2$ (Fig. 4), we infer that effective dd fusion, i.e., $E_M \geq 3$ keV and $Y \geq 10^2$ (inset of Fig. 1) will be realized for Coulomb explosion of $(D_2O)_n$ heteronuclear clusters with $R_0 \simeq 12$ Å.

In contrast to homonuclear clusters, the $(D_2O)_n$ clusters do not exhibit saturation of E_M vs I for the intensity range $I = 10^{17}-2 \times 10^{18}$ W/cm^{-2}, with the onset of complete outer ionization for the smaller clusters being realized at lower I values, below the range employed in the simulations. The cluster size dependence E vs R_0^2 is portrayed in Fig. 4, where we have also included the kinetic energies of the periphery ions $E(R_0) \propto R_0^2$, calculated from Eq. (2). The simulation data approximately obey the CSE $E_M \propto R_0^2$ (Fig. 4). The E curve lies below the $E(R_0)$ curve for $I = 10^{17}$ W/cm^{-1} and above it for the very high laser power of $I = 2 \times 10^{18}$ W/cm^{-2}, which is experimentally accessible [14]. The relation $E < E(R_0)$ can be realized from the nonvertical character of ionization both for heteronuclear and homonuclear clusters. On the other hand, the situation $E > E(R_0)$ is a special feature of heteronuclear clusters. It originates from inner deuterons, which can get higher energy than the periphery deuterons, leaving them behind during the cluster Coulomb explosion. This over-running effect is exhibited in the simulations. Because of the presence of high-energy inner deuterons, the energy distribution of the product D^+ ions from the heteronuclear clusters is shifted to high energy. In Fig. 5 we present the D^+ energy distributions $P(E)$ from $(D)_n$ and $(D_2O)_m$ clusters. The $P(E)$ curve for D^+ from $(D_2O)_n$ is peaked at high energies; e.g., for $(D_2O)_{2171}$ ($R_0 = 25$ Å) about 50% of the D^+ energies fall in the narrow and high-energy interval $E = 8.4-10.1$ keV. This energy distribution, manifesting kinematic effects (with $\eta = 1.33$) is in marked contrast with the broad $P(E)$ curve from $(D)_n$ clusters (Fig. 5). This kinetic energy shift and narrow distribution at high E for heteronuclear clusters facilitates dd fusion.

Our analysis and simulations of multielectron outer ionization and Coulomb explosion demonstrate that the

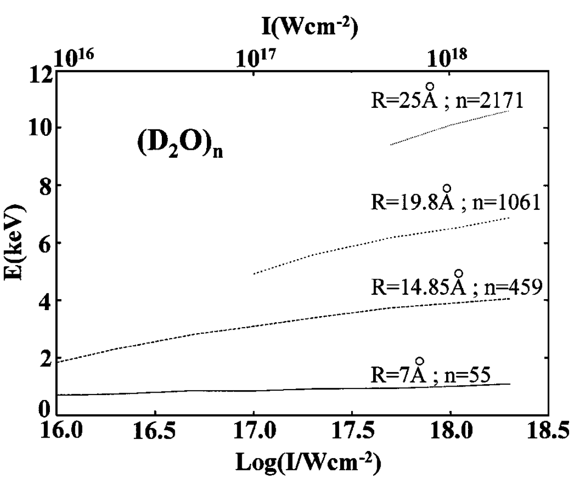

FIG. 3. Simulations of Coulomb explosion of $(D_2O)_n$ clusters, showing the dependence of the maximal D^+ energies on the laser intensity. Cluster sizes are marked on the curves.

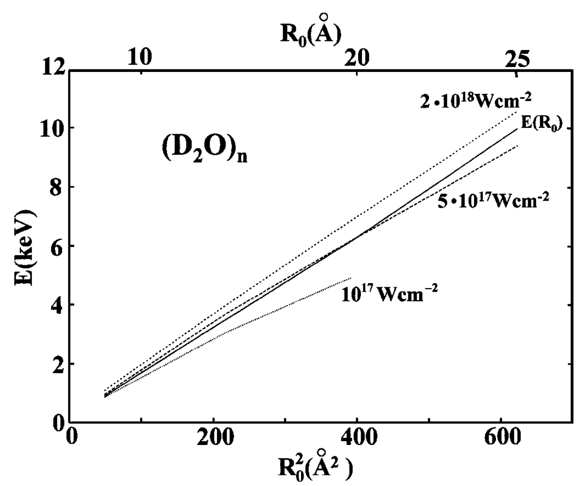

FIG. 4. The dependence of the D^+ maximal energy from the Coulomb explosion $(D_2O)_n$ clusters on R_0^2. The numbers on the dashed curves represent the laser intensities. The solid line represents $E(R_0)$, Eq. (2).

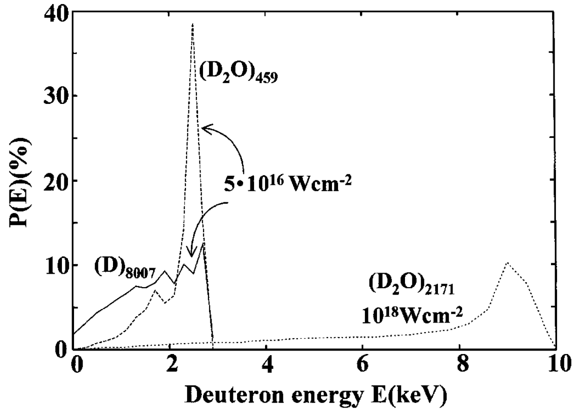

FIG. 5. The deuteron energy distribution in the Coulomb explosion of $(D_2O)_n$ ($n = 450, 2171$) and $(D)_n$ ($n = 8007$) clusters. $P(E)$ is presented as percents per the energy interval of 0.2 keV. The numbers on the curves represent the laser intensity.

deuterium containing heteronuclear clusters, i.e., $(D_2O)_n$, have some important advantages as a source of energetic deuterons, as compared to the homonuclear pure deuterium clusters. This is manifested by an increased D^+ maximal kinetic energy released from moderately small heteronuclear clusters, e.g., 12 Å for $(D_2O)_n$ as compared to 40 Å for $(D)_n$ as a D^+ source ($E = 3.0$ keV) for *dd* fusion, and by the large proportion of high-energy deuterons due to a considerably more favorable energy distribution in the Coulomb explosion of heteronuclear clusters.

[1] J. Purnell, E. M. Snyder, S. Wei, and A. W. Castleman, Jr., Chem. Phys. Lett. **229**, 333 (1994).
[2] T. Ditmire, J. W. G. Tisch, E. Springate, M. B. Mason, N. Hay, R. A. Smith, J. Marangos, and M. H. R. Hutchinson, Nature (London) **386**, 54 (1997).
[3] T. Ditmire, E. Springate, J. W. G. Tisch, Y. L. Shao, M. B. Mason, N. Hay, J. P. Marangos, and M. H. R. Hutchinson, Phys. Rev. A **57**, 369 (1998).
[4] M. Lezius, S. Dobosh, D. Normand, and M. Schmidt, Phys. Rev. Lett. **80**, 261 (1998).
[5] J. Zweiback, R. A. Smith, T. E. Cowan, G. Hays, K. B. Wharton, V. P. Yanovsky, and T. Ditmire, Phys. Rev. Lett. **84**, 2634 (2000).
[6] I. Last and J. Jortner, Phys. Rev. A **62**, 013201 (2000).
[7] T. Ditmire, Phys. Rev. A **57**, R4094 (1998).
[8] I Last, I. Schek, and J. Jortner, J. Chem. Phys. **107**, 6685 (1997).
[9] J. Jortner, Z. Phys. D **24**, 247 (1992); J. Jortner, J. Chim. Phys. **92**, 205 (1995); Z. Phys. Chem. **184**, 283 (1994).
[10] H. S. Massey and H. B. Gilbody, *Electronic and Ionic Impact Phenomena* (Oxford University Press, New York, 1974), Vol. 4.
[11] I. Last and J. Jortner, Phys. Rev. A **60**, 2215 (1999).
[12] A. Talebpour, K. Vijayalakshmi, A. S. D. Bandrauk, T. T. Nguyen-Dang, and S. L. Chin, Phys. Rev. A **62**, 042708 (2000).
[13] L. A. Artsimovich, *Controlled Thermonuclear Reactions* (Gordon and Breach, New York, 1964).
[14] G. A. Mourou, Ch. P. J. Barty, and M. D. Perry, Phys. Today **51**, No. 1, 22 (1998).