

**Table 1. Energetics and dynamics of Coulomb explosion of deuterium containing homonuclear  $(D_2)_n$  clusters and heteronuclear  $(A_k^{q_A} B_\ell^{q_B})_n$  or  $(A_k^{q_A} B_\ell^{q_B} C_p^{q_C})_n$  clusters at  $I_M = 10^{18} \text{ W}\cdot\text{cm}^{-2}$**

Cluster	$\rho_{\text{mol}},^* \text{ \AA}^{-3}$	$q_{\text{mol}} \text{ or } q_B^\dagger$	$Z, \text{ eV SIM}^\ddagger;$ <b>EML</b> <sup>§¶</sup>	$\kappa \text{ SIM}^\ddagger;$ <b>EML</b> <sup>§¶</sup>	$a, \text{ fs}^{-1} \text{ SIM};$ <b>EML</b> <sup>¶  </sup>
$(D_2)_n$	0.025	2	12.5; 13.6	0.61; 0.60	0.16; 0.17
$(CD_4)_n$	0.016	8	42.5; 46.7	0.70; 0.60	0.27
$(DI)_n$	0.013	22	115; 165	0.80; 0.83	0.50; 0.45
$(CD_3I)_n$	0.010	26	130; 181	0.80; 0.83	

Simulation data (SIM) are compared with the results of the electrostatic model (EML). The cluster initial radius is related to  $n$  by  $R_0 = (3n/4\pi\rho_{\text{mol}})^{1/3}$ .

\*Initial molecular density of molecular ion.

†Ion charge  $q_{\text{mol}} = kq_A + \ell q_B + pq_C$  for cases A and B, and  $q_{\text{mol}} = \ell q_B + pq_C$  for ECLHH, where  $q_I = 22$  is an average charge in the size domain  $n = 1061\text{--}2171$ , and  $q_C = 4$  for  $(CD_3I)_{2171}$ .

‡ $E_M(n) = Zn^{2/3}$  and  $\kappa = E_M(n)/E_{\text{av}}(n)$ , with  $Z$  and  $\kappa$  being independent of  $n$ .

§See Fig. 3.

¶See text. For the ECLHHs, we neglect a weak cluster size dependence of  $Z$ , due to the dependence of  $q_I$  on  $n$ , which arises from ignition and screening effects on inner ionization [Last, I. & Jortner, J. (2004) *J. Chem. Phys.* **120**, 1336–1347; Last, I. & Jortner, J. (2005) *Proc. Natl. Acad. Sci. USA* **102**, 1291–1295].

||From the time dependence of the first moment of the distribution of the light ions,  $\langle R \rangle = \langle R \rangle_0 = a(t - t_{\text{onset}})$ .