# Tunneling channels in strong field enhanced ionization of diatomic molecules

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**Abstract:** We theoretically demonstrated two new ionization channels through which the electron can be released either from the down-field or up-field site of diatomic molecules. Our finding provides a comprehensive physical picture of molecular enhanced ionization.
**OCIS codes:** (320.2250) Femtosecond phenomena; (260.3230) Ionization ; (270.6620 ) Strong-field processes

Tunneling ionization of atoms or molecules is the doorway step and at the core of nearly every process in strong laser fields, from high harmonic generation to correlated multiple ionization and so on. Understanding the ionization dynamics is of essential importance for probing and controlling the electron dynamics in these processes. Great efforts have been made over the past several decades. Nevertheless, because the molecules have more degrees of freedom, the underlying physics is richer and the ionization dynamics is still not completely clear. It has been demonstrated that when the molecule is stretched to a critical internuclear distance the ionization probability sharply increases, which is called enhanced ionization (EI) [1-3]. An intuitive physical explanation is that the electron wave packet is directly freed from the up-field site (DIU). Even through this explanation has been widely used, the cornerstone of the intuitive physical picture, i.e., the tunneling site, is still under debate and confusing. Some experimental works even contradict each other [4,5]. For instance, Betsch *et al*'s [4] experiment implies that the electron is preferentially emitted from the down-field site in the two-color field. However, the recent experimental result for the dimmer ArXe by Wu *et al.* shows that the ionization more easily happens at the up-field site in elliptically polarized field. Because the intuitive physical picture is based on the quasi-static theory, lacking a perspective on the dynamics of ionization processes, the physical dynamics of molecular EI becomes a long-standing issues and a subject of hot debate.

In this work, we investigate the electron dynamics and the tunneling site by examining time evolution of the electron density and ionization rate with numerically solving time-dependent Schrodinger equation (TDSE). A more comprehensive physical picture is established for EI dynamics of diatomic molecules. It is demonstrated that the widely-used DIU physical picture of EI is incomplete. Besides the DIU ionization channel, we find another two new ionization channels, the field-induced excitation with subsequent ionization from the down-field site (ESID), and the up-field site (ESIU). Through these two channels, the electron can be released from the down-field and up-field site of diatomic molecules, respectively. The contributions from these channels depend on the asymmetry and internuclear distance of the molecules. These findings provide a more comprehensive understanding for the long-standing issue about EI of diatomic molecules.

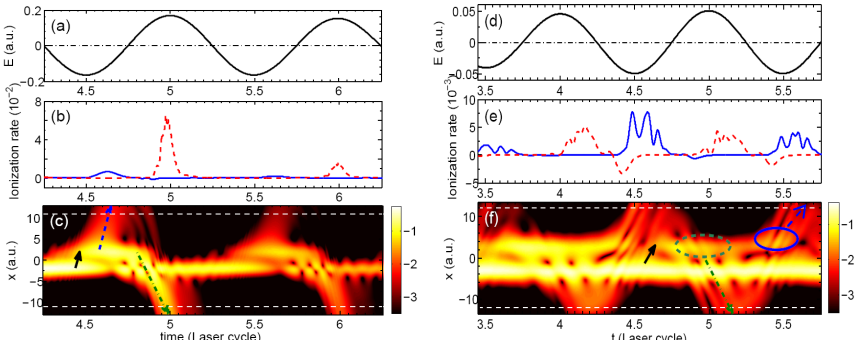


Fig.1 (a) The laser electric field. (b) Ionization rate from the left (red) and right (blue) sides as a function of time. (c) Electron density as a function of time and the coordinate x. Molecule with large asymmetry at R=4 a.u. (d),(e) and (f) are same to (a),(b) and (c), but for the molecule with small asymmetry at R=6 a.u..

A two-dimensional TDSE model is adopted in our simulation. Since this work is intended to explore a general effect, rather than to model a specific experiment, we consider a generic model diatomic molecule aligned along the electric field vector of the linearly polarized light. Like Refs.[4,5,6], to clearly indentify the tunneling site, we simulate the ionization of polar diatomic molecules. We assume that the core with deep potential well is localized at

the left side (–R/2, 0) and the other core with shallow potential well is localized at the right side (R/2, 0), where R is the internuclear distance. In order to investigate the role of molecular asymmetry, we simulate two molecules. One has a large asymmetry like $HeH^{2+}$[6]. The other one has a smaller asymmetry, like ArXe[5]. In our work, the laser wavelength is 800nm.

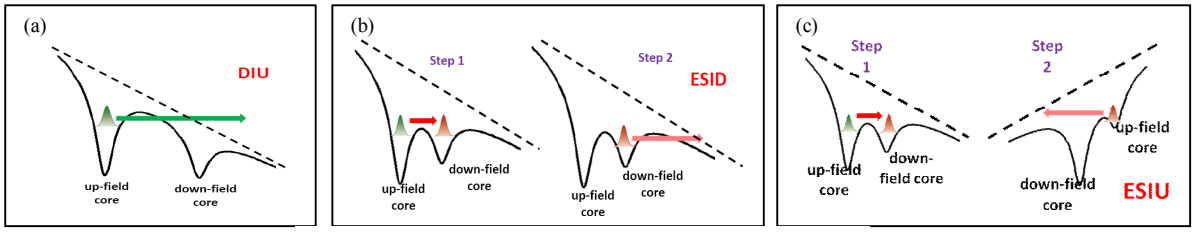


Fig.2 Sketch of ionization channels of DIU, ESID and ESIU.

Figures 1 (a)-(c) and (d)-(f) show the ionization for the molecules with large and small asymmetry, respectively. We first analysis the molecule with large asymmetry. As shown in Fig. 1(b) and (c), the dominant ionization burst is from the left side around t=5.0T, where T is the laser period and the electric field is positive. There are also some electron wave packets escaping away from the right side with low probabilities around t=4.65T and t=5.65T, and from the left side around t=6.0T. A more clearly reveal of the electronic dynamics can be seen from Fig. 3(c). At t=0, the electron wave packet is dominantly localized at the left core. At t=4.45T, some electron population is firstly excited to the right core [see the black arrow]. A short time later, at t=4.6T a small part of the excited population leaves from the right core and then ionized [see the blue arrow]. At this time the electric field is still negative and thus the right core is down-filed. Therefore, the electron escapes away from the down-field site by this process. Furthermore, more excited population remains localized at the right core. When the electric field becomes positive and the right core is promoted to the up-field site, the excited population quickly tunnels through the inner potential barrier to the continuum around t=5.0T [see the green arrow], which corresponds to the highest ionization peak in Fig. 1(b). In this channel the electron is emitted from the up-field site. Clearly, these ionization processes cannot be explained with the well-known DIU. The differences are illustrated in Fig. 2. For DIU, the electron wave packet is directly freed through the inner barrier and emitted from the up-field site [see Fig.2(a)]. The ionization channels shown in Fig. 1 are two-step processes. The first step is that the electron population located at the left core is excited to the right core when the electric field is negative. Then the excited electron wave packet can be ionized by two paths. One path is that the excited electron wave packet tunnels through the right outer barrier from the down-field site when the electric field is negative [see Fig. 2(b)]. We call this channel *field-induced excitation with subsequent ionization from the down-field site (ESID).*The other path is that the excited electron wave packet stays until the electric field reverses and then tunnels through the inner potential barrier from the up-field site [see Fig. 2(c)], which is called *field-induced excitation with subsequent ionization from the up-field site (ESIU).*

One can understand the ionization dynamics of small asymmetric molecules by the same way. As shown in Fig. 1 (f) , a part of electron population is excited to the right core at t=4.6T [see the black arrow]. Then the electric field turns positive at t=4.75T and within the subsequent positive half-cycle, a part of excited electron population tunnels through the inner barrier from the left side [see the green arrow]. After the electric field reverses again at t=5.25T, the right core is lowered to the down-field site. The residual excited population localized at the right core tunnels through the right outer barrier to the continuum around t=5.5T [see the blue arrow]. These two ionization at t=5.1T and 5.5T correspond to ESIU and ESID channels, respectively. Moreover, one can see from Fig. 1 (e) that ESID is dominant over ESIU for small asymmetric molecule, i.e., the excited electron population is more likely ionized from the down-field site, which is opposite to the case of the molecule with large asymmetry and also in contradiction with the DIU physical picture. These results indicate that the well-known DIU physical picture is too simple. The electron also can be preferentially emitted from either the up-field site or down-field site through ESIU and ESID channels. Their contributions depend on the molecular structure and internuclear distance. These simulation results qualitatively explain the debate of tunneling site in experiments [4,5] and provide a more comprehensive understanding for the long-standing issue about EI of diatomic molecules.

## References

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