



Research paper

# Electric field induced dissociation of a confined hydrogen molecule

Gaia Micca Longo<sup>a,\*</sup>, Savino Longo<sup>a,b</sup><sup>a</sup> Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via Orabona 4, 70125 Bari, Italy<sup>b</sup> Istituto per la Scienza e Tecnologia dei Plasmi - Consiglio Nazionale delle Ricerche, Sezione di Bari, Via Amendola 122/D, 70125 Bari, Italy

## ARTICLE INFO

## Keywords:

Hydrogen  
Molecular dissociation  
Electric field  
Confinement  
DMC

## ABSTRACT

The effect of a static electric field ionization on the neutral hydrogen molecule  $H_2$  confined in a spherical potential well is studied, as a simple model for the chemical activation of molecular species in a medium. Quantum diffusion Monte Carlo is employed with complete account of electron correlation. Field-induced ionization and dissociation are discussed, for different values of the confinement radius and electric field strength. This study allows to highlight the mechanism of electric field initiation of chemical reactions in fluids at different pressures, without the details of a specific chemical environment.

## 1. Introduction

In the last decades, a great interest in effects of intense electric fields on molecular substances or liquid mixtures has arisen [1,2]. The electric field induces chemical activation of the mixture, i.e. radical and ion formation, that starts a sequence of re-association reactions. The Miller-Urey experiment [3–5] is one of the most famous applications: electric discharges fired into a gaseous mixture, with a chemical composition compatible with the mid-20th-century ideas of a primordial reducing atmosphere, does produce life molecules, such as amino acids [6]. Indeed, the neutral hydrogen molecule ( $H_2$ ) is one of the main components of the primordial reducing atmospheres, and one of the main components of the mixture used in the Miller-Urey experiments.

Although some details of this approach have been criticized [7,8], it allows to gain some useful insight into the chemical activation process.

The molecular details of the substances and mixtures considered in the various simulations make each of these systems peculiar, leading to a combinatorial explosion of studies. This does not help the understanding the principles of chemical kinetics induced by an electric field.

One way of highlighting the fundamental aspects of the chemical activation process by a strong electric field is to replace the actual chemical surroundings, due to molecules, with a physical exemplification, namely a simpler representation through a potential well.

Indeed, spatially confined quantum systems have become the subject of increasing attention because when a very high pressure is exerted on a system, its chemical and physical properties can change drastically compared to the cases of corresponding unconfined systems [9,10]. The numerous studies of confined systems provided many useful insights

related to chemical–physical or nano-electronic systems, such as solid state physics [11–14], quantum dots and quantum wells [15–18], zeolites [19], carbon nanotubes [20].

In the study of confined molecules, special attention has been devoted to the neutral hydrogen molecule  $H_2$ , using mostly a variational approach when the molecule is confined into a prolate spheroidal box [21–24]. In order to simulate the pressure effects on  $H_2$  located in the cage, molecular hydrogen endohedrally confined in  $H_{20}$  and  $H_{60}$ -fullerene-like cavities have been studied using density functional theory [25,26]. Pang [27] calculated the exact equilibrium ground-state energy and bond length of a hydrogen molecule confined in a spheroidal using diffusion Monte Carlo (DMC). A complete account for theoretical studies and wide range of applications of confined atomic and molecular systems can be found in [28,29] and references therein.

The intense field ionization and dissociation of the  $H_2^+$  molecule in short-pulse laser has been studied [30–32]. Recent works focus on the effects of a static electric field on a single confined hydrogen atom, as an ideal system for studying the ionization of the atom itself in static conditions [33,34].

In this work, the  $H_2$  molecule confined into a spherical potential well is studied using the DMC method: the effect of a static electric field ionization is investigated, as a simple model for the chemical activation of molecular species in a medium.

Our model shows that, without any specific detail of the chemical environment in which the hydrogen molecule is immersed, an appropriate combination of confinement and electric field produces the molecule dissociation. In this way, a simple mechanism to produce radicals in this kind of systems emerges. Moreover, it is possible to

\* Corresponding author.

E-mail addresses: [gaia.miccalongo@uniba.it](mailto:gaia.miccalongo@uniba.it) (G. Micca Longo), [savino.longo@uniba.it](mailto:savino.longo@uniba.it) (S. Longo).<https://doi.org/10.1016/j.cplett.2024.141643>

Received 23 July 2024; Received in revised form 5 September 2024; Accepted 15 September 2024

Available online 16 September 2024

0009-2614/© 2024 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

describe the combined effects of pressure variations and electric field.

## 2. Method

DMC method is based on the similarity between the imaginary time Schrödinger equation and a generalized diffusion equation, that can be solved using a stochastic calculation and simulating a random walk [35].

The diffusion process of numerous “walkers” in the phase space is simulated. A walker is a mobile mathematical point in a set  $\{R_i\}$  of phase coordinates  $R$  in a  $3N$ -dimensional space, where  $N$  is the number of physical electrons in the system (two, in this case of study); the number of walkers  $M$  is an integer numerical variable,  $M \sim 10^3$ . The evolution in the phase space is performed by repeated application of the short-time diffusion–reaction propagator

$$G(\mathbf{r} \leftarrow \mathbf{r}', \tau) \approx (2\pi\tau)^{-\frac{3N}{2}} \exp\left[-\frac{(\mathbf{r} - \mathbf{r}')^2}{2\tau}\right] \exp\left[\frac{-\tau(V(\mathbf{r}) - V(\mathbf{r}') - 2E_T)}{2}\right] \quad (1)$$

where  $\tau$  is the numerical step and  $V$  is the potential energy. The first exponential term represents the diffusion equation, while the second exponential term is the so-called birth–death algorithm, according to which the walkers multiply in low potential regions and disappear in high potential ones.  $E_T$  is the energy offset that controls the walker total population and is adapted by a relaxation method until the numerical equilibrium of walker population is reached:

$$E_{T_i} = E_{T_{i-1}} + \alpha \ln\left(\frac{M_{av,i}}{M_i}\right) \quad (2)$$

where  $\alpha$  is a small positive parameter,  $E_{T_i}$  and  $E_{T_{i-1}}$  are the energy values at time step  $i$  and  $i-1$ ,  $M_{av,i}$  and  $M_i$  are the average number of walkers and the number of actual walkers at time step  $i$ .

The DMC method is used here in its unbiased version, with no *a priori* functions (importance sampling). Furthermore, a numerically efficient technique for generating the walker diffusion is employed, replacing the diffusion factor in equation (1) with a uniform distribution in a cube centered into  $\mathbf{r}$  and with edge length  $2\sqrt{3}\tau$ , to match the variance of the gaussian propagator [36].

DMC can handle only positive distributions, so dealing with a many electron wavefunction leads to a series of problems. However, in the case of two-electron systems, an unrestricted, six-dimensional wavefunction  $\psi(r_1, r_2)$  of the singlet ground state can be calculated directly. This means that the electron correlation is accounted exactly: no expansion of the wavefunction  $\psi$  is needed, and no function database needs to be included. Therefore, DMC method is applied to the confined  $H_2$  by simulating a six-dimensional phase space. The use of the Cartesian coordinates represents a straightforward advantage of the present DMC code, since a change of the dimensionality of the system can be realized with very few modifications to the calculation program.

Calculations presented in this work have been performed using the open-source program *DMC\_Basic* (see Data Availability): this is a Fortran-language standard DMC program that allows to find the ground state and symmetry-selected excited states of one- and two-electron systems confined in potential wells of any shape, with a very limited number of numerical parameters to be optimized (typically: the energy offset  $E_T$ , the time step  $\tau$  and the number of walkers).

The  $H_2$  Hamiltonian, in atomic units, can be written as:

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_a|} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_b|} - \frac{1}{|\mathbf{r}_2 - \mathbf{r}_a|} - \frac{1}{|\mathbf{r}_2 - \mathbf{r}_b|} + \frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} - \mathcal{E}(z_1 + z_2 - z_a - z_b) \quad (3)$$

The external electric field  $\mathcal{E}$  is applied along the negative direction of the  $z$  axis; the Coulomb energy term goes to infinite outside the confinement barrier of dimension  $c$  (Fig. 1).

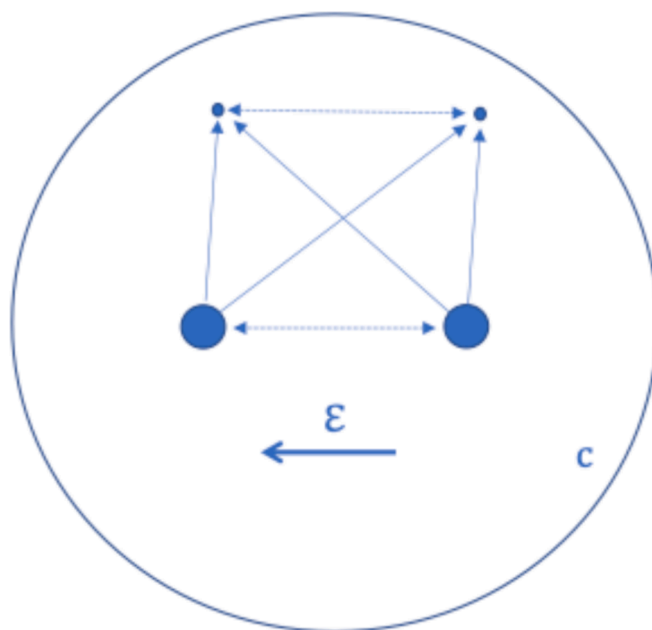


Fig. 1. Schematic drawing of the interactions in the  $H_2$  molecule confined in a spherical cavity of dimension  $c$ , with an applied electric field  $\mathcal{E}$ .

The calculations are repeated for different positions of the two nuclei, with a reduced dimensionality assumption: the nuclei move on the same line through the center of the dielectric well, and the electric field is applied in the same direction. This provides an initial set of potential energy surfaces (PESs) as a function of two coordinates that fully characterize the system in reduced dimensionality.

Calculations are performed within the Born–Oppenheimer approximation: the nuclei are modeled as classical point-like source of Coulomb potentials, placed in different locations inside the potential well. Atomic units (a. u.) are used throughout.

## 3. Results

In this section, we present results concerning the spherically confined hydrogen molecule, with and without an external static electric field, in order to study the effects of this electric field on a confined molecular system.

The DMC calculations are performed with an imaginary time step equal to  $3 \times 10^{-3}$ , totaling  $10^6$  time steps, during which the energy is updated and time-averaged, using  $2 \times 10^3$  walkers in the six-dimensional configuration space.

Fig. 2 shows potential energy curves of an  $H_2$  molecule confined in spheres of different radius  $c$ . No electric field is applied.

Results show that, in the absence of an electric field, the potential well can emulate the effect of a high pressure in the liquid phase in a simplified way, and decreasing the radius of the potential well shows a reduction in the internuclear distance and an increase in energy. Fig. 2 demonstrates the effects due to compression, already discussed in previous work for the  $H_2^+$  system [37–39]: as the nuclei are close to the inner surface of the spherical potential well, an increase in total energy is observed, due to the additional nodal surface in the atomic wavefunction.

Figs. 3 and 4 show the PESs of the  $H_2$  molecule confined in a sphere of radius  $c = 3$  a. u. and  $c = 5$  a. u., respectively, when an external electric field of different values ( $\mathcal{E} = 0.1$  a. u.,  $\mathcal{E} = 0.5$  a. u. and  $\mathcal{E} = 1$  a. u.) is applied along the  $z$  direction. Energy is plotted as a function of the  $z_a$  of nucleus  $a$  coordinate and the internuclear distance  $z_b - z_a$ , while the nuclei are displaced along the  $z$  axis.

A weak electric field (atomic unit fraction) shows effects that can be

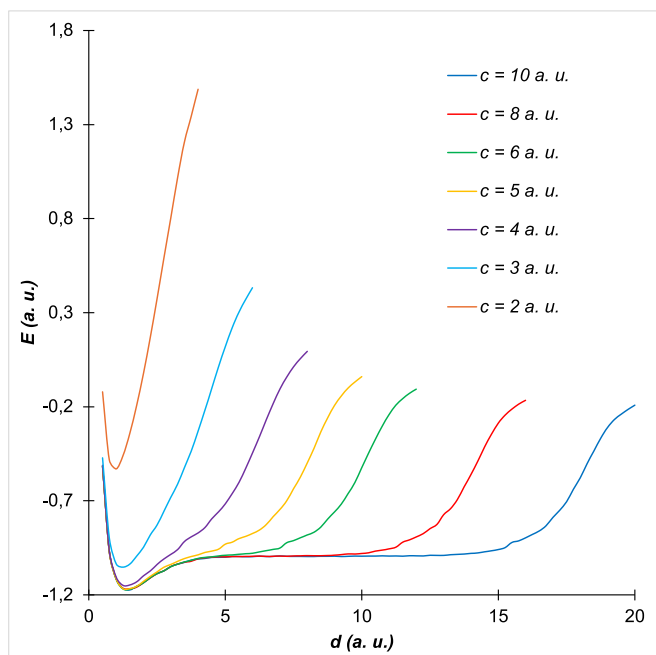


Fig. 2. Energy of a free hydrogen molecule  $H_2$  as a function of the internuclear distance  $d$ , for different spherical confinement dimension  $c$ .

linked to molecular ionization. This direct dissociation effect associated with partial ionization induced by the electric field is compatible with the effects observed in *ab-initio* simulations where a strong pulsed electric field induces chemical activation of the mixture. With a more intense electric field (1 a. u.), both nuclei are strongly pushed in the direction of the electric field and thus tend to reconstitute a very close and, only in the presence of the dielectric barrier, strongly bonded system.

#### 4. Discussion

The tighter confinement  $c = 3$  a. u. (Fig. 3) significantly limits the molecular electronic clouds, and this situation necessarily requires external works. Consequently, the system is under pressure, namely degenerative quantum pressure, that does not depend on the temperature. It can be estimated from the thermodynamic relation [40]:

$$p = - \left( \frac{\partial E}{\partial V} \right)_T \quad (4)$$

where  $E$  is the energy,  $V$  the volume of the confining sphere,  $T$  the temperature, here  $T = 0$ . In this case,  $p = \text{Mbar}$ , a pressure of geophysical significance [41] and well accessible to laboratory measurement using a diamond anvil cell [42].

The small internuclear distance corresponding to the minimum in two cases ( $c = 3$  a. u.,  $\mathcal{E} = 0.1$  a. u.,  $z_b - z_a = 1.35$  a. u.,  $E = -1.1$  a. u.;  $c = 3$  a. u.,  $\mathcal{E} = 1$  a. u.,  $z_b - z_a = 1.20$  a. u.,  $E = -5.2$  a. u.) shows that the  $H_2$  molecule has indeed been compressed, and that the increased electron density compensates for the internuclear repulsion. In this situation, the effect of the external electric field is reduced, and this is understandable from a physical point of view: the electric field never produces a significant separation of the nuclei. This behavior of the compressed molecule can be seen as an ionization effect due to the pressure itself, a well-known effect in the study of hydrogen under pressure, for example, in the interior of the large gaseous planets [43]. This also shows that dissociation is hindered by the increase in pressure, that can be seen as a consequence of Le Chatelier's principle [40].

The larger confinement dimension ( $c = 5$  a. u., Fig. 4) roughly corresponds to the internuclear distance in liquid  $H_2$ : therefore, the confinement represents a simplified model of the chemical environment of  $H_2$  at low temperature and atmospheric pressure. In this case, the effect of the electric field is much more evident. The more intense electric field ( $\mathcal{E} = 1$  a. u.) essentially leads to ionization of the molecule: electrons are no longer bound by the nuclear potential and are displaced in opposite direction of the electric field, while remaining confined by the confinement sphere. For the same reasons, the nuclei are pushed in

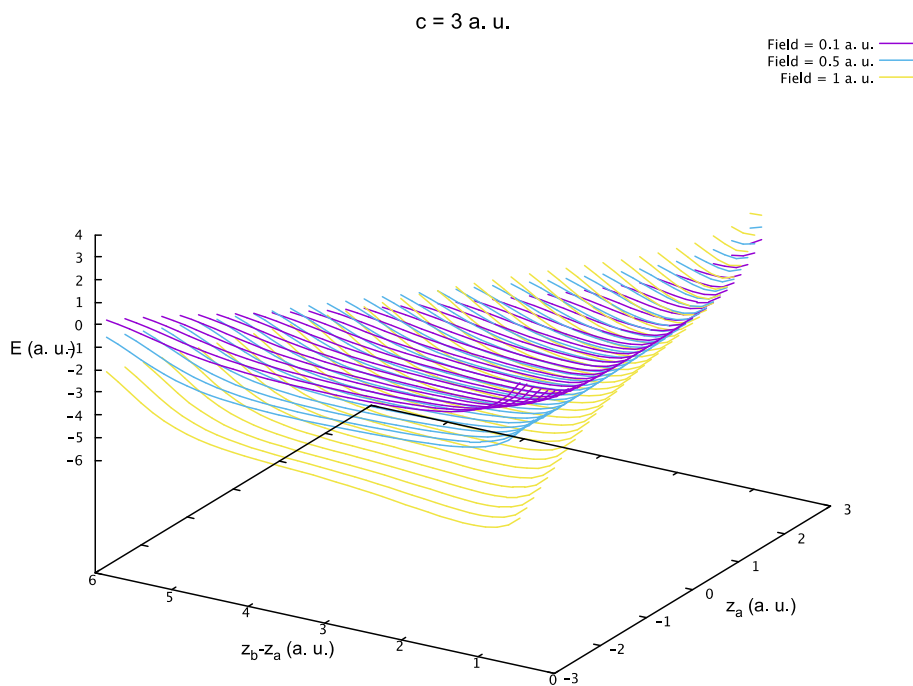
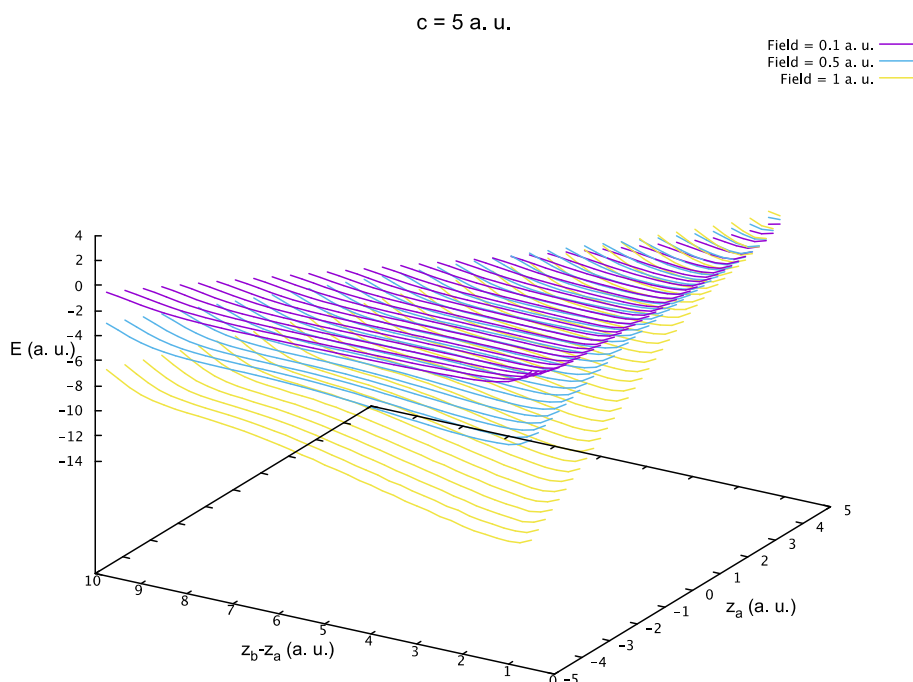


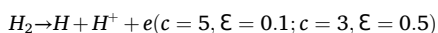
Fig. 3. Potential energy surfaces of a hydrogen molecule  $H_2$  inside a sphere of radius  $c = 3$  a. u., corresponding to a pressure of 0.76 Mbar: energy  $E$  as a function of the internuclear distance  $z_b - z_a$  and the nucleus coordinate  $z_a$ , while the nuclei are displaced along the  $z$  direction of the confinement sphere. Three values of the electric field are reported:  $\mathcal{E} = 0.1$  a. u. (purple),  $\mathcal{E} = 0.5$  a. u. (blue),  $\mathcal{E} = 1$  a. u. (yellow).



**Fig. 4.** Potential energy surfaces of a hydrogen molecule  $H_2$  inside a sphere of radius  $c = 5 \text{ a. u.}$ , close to an environment under standard conditions: energy  $E$  as a function of the internuclear distance  $z_b - z_a$  and the nucleus coordinate  $z_a$ , while the nuclei are displaced along the  $z$  direction of the confinement sphere. Three values of the electric field are reported:  $\mathcal{E} = 0.1 \text{ a. u.}$  (purple),  $\mathcal{E} = 0.5 \text{ a. u.}$  (blue),  $\mathcal{E} = 1 \text{ a. u.}$  (yellow).

the direction of the electric field and, assuming the reduced dimensionality, align themselves near the potential barrier and move closer until the external electric field is balanced with the internuclear repulsion. Consistently, the equilibrium distance between the nuclei is  $\mathcal{E}^{-1/2}$ . Again, this is a strongly bound system, but somewhat artificial: it is a balance between the barrier effect and the electric field effect. Indeed, the electric field strength in this case is probably unrealizable in an experiment.

The case  $c = 5 \text{ a. u.}$  and  $\mathcal{E} = 0.1 \text{ a. u.}$  is the most interesting one. From the purple PES in Fig. 4, the most stable situation ( $E = -1.22 \text{ a. u.}$ ) is obtained when the two nuclei are relatively far apart ( $z_b - z_a = 6.25 \text{ a. u.}$ ), at a distance significantly greater than the internuclear distance of the unperturbed molecule. A similar situation appears for a tighter confinement  $c = 3 \text{ a. u.}$ , but for a higher electric field ( $\mathcal{E} = 0.5 \text{ a. u.}$ ,  $z_b - z_a = 3.3 \text{ a. u.}$ ,  $E = -2.2 \text{ a. u.}$ ). The process



can be seen as dissociative ionization induced by the electric field. This shows a chemical activation of the molecule by dissociation, thereby radical formation. Our calculation also shows that molecular dissociation induced by an electric field requires a stronger field if the liquid is more compressed. This result describes, without the need for chemical detail, the chemical activation mechanism in typical *ab-initio* simulations triggered by intense electric fields. Moreover, this dissociation is inevitably associated with partial ionization, which is confirmed by the fact that one of the nuclei is in contact with the confining wall, indicating an almost zero local electron density. This is an important insight, since, in a real chemical mixture, chemical activation due to an electric field is typically associated with ionization, i.e. plasma formation, where a part of the molecular electrons behave like a free electron gas. The plasma formation cannot be described in detail under the physical assumptions of this work, as it rather requires a dynamic calculation of reactive quantum scattering [44]. At the same time, the ionization-dissociation process described here has its own interest as a reversible and static phenomenon. The simulation describes instead the ionization of the gas under the assumptions in which it is formulated. A different

formulation of boundary conditions, for example like those used in condensed matter physics, with spatially tessellating potential barriers, could be used to describe the ionization phenomenon more accurately.

## 5. Conclusions

A quantum Monte Carlo calculation has been set up to simulate a single  $H_2$  molecule under the effect of a variable static electric field, while confined into a spherical potential well. This system is intended to describe the chemical activation of a molecular fluid under the effect of the electric field, a scenario that has been object of many studies in the recent years. The molecule is characterized by its PESs, determined by displacing the classical nuclei.

For a confinement radius compatible with typical intermolecular separations, and moderate field strength, an equilibrium configuration with widely spaced nuclei is achieved, that can be interpreted as molecular dissociation due to the field. At high pressure, this mechanism required a higher field strength. These results provide insight on how an intense electric field affects a chemical system in various applications potentially including the prebiotic chemistry through the Miller-Urey experience.

## CRediT authorship contribution statement

**Gaia Micca Longo:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Savino Longo:** Writing – review & editing, Writing – original draft, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

Data will be made available on request.

## Acknowledgements

The authors acknowledge PNRR MUR project PE0000023-NQSTI (National Quantum Science and Technology Institute) and PRIN2022 MUR project P20224C3NJ Brave New Worlds.

## References

- [1] P. Umari, A. Pasquarello, Ab initio molecular dynamics in a finite homogeneous electric field, *Phys. Rev. Lett.* 89 (15) (2002) 157602.
- [2] A.M. Saitta, F. Saija, P.V. Giaquinta, Ab initio molecular dynamics study of dissociation of water under an electric field, *Phys. Rev. Lett.* 108 (20) (2012) 207801.
- [3] S.L. Miller, A production of amino acids under possible primitive earth conditions, *Science* 117 (3046) (1953) 528–529.
- [4] S.L. Miller, Production of some organic compounds under possible primitive earth conditions, *J. Am. Chem. Soc.* 77 (9) (1955) 2351–2361.
- [5] S.L. Miller, H.C. Urey, Organic compound synthesis on the primitive Earth: Several questions about the origin of life have been answered, but much remains to be studied, *Science* 130 (3370) (1959) 245–251.
- [6] A.M. Saitta, F. Saija, Miller experiments in atomistic computer simulations, *Proc. Natl. Acad. Sci.* 111 (38) (2014) 13768–13773.
- [7] J.L. Bada, H.J. Cleaves, Ab initio simulations and the Miller prebiotic synthesis experiment, *Proc. Natl. Acad. Sci.* 112 (4) (2015) E342–E.
- [8] S. Longo, The spark of life: discharge physics as a key aspect of the Miller-Urey experiment, *Front. Phys.* 12 (2024) 1392578.
- [9] J.R. Sabin, E.J. Brändas, *Advances in quantum chemistry: theory of confined quantum systems*, Academic, Waltham, Vol. 2009, p. 57.
- [10] K.E. Gubbins, Y.C. Liu, J.D. Moore, J.C. Palmer, The role of molecular modeling in confined systems: impact and prospects, *PCCP* 13 (1) (2011) 58–85.
- [11] V.R. Belosludov, T.M. Inerbaev, R.V. Belosludov, Y. Kawazoe, Polaron in a one-dimensional C 60 crystal, *Phys. Rev. B* 67 (15) (2003) 155410.
- [12] Y.X. Ren, T.Y. Ng, K.M. Liew, State of hydrogen molecules confined in C60 fullerene and carbon nanocapsule structures, *Carbon* 44 (3) (2006) 397–406.
- [13] C.Y. Lin, Y.K. Ho, Photoionization of endohedral atoms in fullerene cages, *Few-Body Syst.* 54 (1) (2013) 425–429.
- [14] A. Krachmalnicoff, R. Bounds, S. Mamone, S. Alom, M. Concistre, B. Meier, R. J. Whitby, The dipolar endofullerene HF@ C60, *Nat. Chem.* 8 (10) (2016) 953–957.
- [15] D. Vasudevan, R.R. Gaddam, A. Trinchi, I. Cole, Core-shell quantum dots: Properties and applications, *J. Alloy. Compd.* 636 (2015) 395–404.
- [16] P. Harrison, A. Valavanis, *Quantum wells, wires and dots: theoretical and computational physics of semiconductor nanostructures*, John Wiley & Sons, Hoboken, United States, 2016.
- [17] D. Munjal, K.D. Sen, V. Prasad, Shape effect on information theoretic measures of quantum heterostructures, *J. Phys. Commun.* 2 (2) (2018) 025002.
- [18] Y. Sun, J.L. Xiao, Qubit coherence effects in a RbCl quantum well with asymmetric Gaussian confinement potential and applied electric field, *The European Physical Journal plus* 135 (7) (2020) 1–9.
- [19] H. Lv, M. Yao, Q. Li, R. Liu, B. Liu, Z. Yao, B. Liu, Insertion of N2 into the Channels of AFI Zeolite under High Pressure, *Sci. Rep.* 5 (1) (2015) 13234.
- [20] B. Trzaskowski, L. Adamowicz, Chloromethane and dichloromethane decompositions inside nanotubes as models of reactions in confined space, *Theor. Chem. Acc.* 124 (2009) 95–103.
- [21] R. Colín-Rodríguez, S.A. Cruz, The hydrogen molecule inside prolate spheroidal boxes: full nuclear position optimization, *J. Phys. B Atomic Mol. Phys.* 43 (23) (2010) 235102.
- [22] R. Colín-Rodríguez, C. Díaz-García, S.A. Cruz, The hydrogen molecule and the H+ 2 molecular ion inside padded prolate spheroidal cavities with arbitrary nuclear positions, *J. Phys. B Atomic Mol. Phys.* 44 (24) (2011) 241001.
- [23] H.D.O. Batael, E. Drigo Filho, Ground-state energy for confined H 2: a variational approach, *Theor. Chem. Acc.* 137 (2018) 1–6.
- [24] S.B. Doma, F.N. El-Gammal, A.A. Amer, Ground-state calculations of confined hydrogen molecule H2 using variational Monte Carlo method, *Mol. Phys.* 116 (14) (2018) 1827–1833.
- [25] J. Soullard, R. Santamaria, S.A. Cruz, Endohedral confinement of molecular hydrogen, *Chem. Phys. Lett.* 391 (1–3) (2004) 187–190.
- [26] O.P. Charkin, N.M. Klimenko, D.O. Charkin, DFT study of molecules confined inside fullerene and fullerene-like cages, *Adv. Quantum Chem.* 58 (2009) 69–114.
- [27] T. Pang, Hydrogen molecule under confinement: Exact results, *Phys. Rev. A* 49 (3) (1994) 1709.
- [28] K.D. Sen, K.D. Sen (Eds.), *Electronic Structure of Quantum Confined Atoms and Molecules*, Springer, Switzerland, 2014, pp. 978–983.
- [29] E. Ley-Koo, Recent progress in confined atoms and molecules: Superintegrability and symmetry breakings, *Revista Mexicana De Física* 64 (4) (2018) 326–363.
- [30] A.D. Bandrauk (Ed.), *Molecules in Laser Fields*, CRC Press, 1993.
- [31] T. Zuo, A.D. Bandrauk, Charge-resonance-enhanced ionization of diatomic molecular ions by intense lasers, *Phys. Rev. A* 52 (4) (1995) R2511.
- [32] G.N. Gibson, M. Li, C. Guo, J. Neira, Strong-field dissociation and ionization of H 2 + using ultrashort laser pulses, *Phys. Rev. Lett.* 79 (11) (1997) 2022.
- [33] G. Micca Longo, D. Giordano, S. Longo, Static field ionization of the spherically confined hydrogen atom, *Int. J. Quantum Chem* 124 (1) (2024) e27249.
- [34] G. Micca Longo, S. Longo, Quantum states and static field ionization of a cylindrical confined hydrogen atom: A diffusion Monte Carlo study, *Int. J. Quantum Chem* 124 (10) (2024) e27392.
- [35] W.M. Foulkes, L. Mitas, R.J. Needs, G. Rajagopal, Quantum Monte Carlo simulations of solids, *Rev. Mod. Phys.* 73 (1) (2001) 33.
- [36] G. Micca Longo, C.M. Coppola, D. Giordano, S. Longo, The unbiased diffusion Monte Carlo: a versatile tool for two-electron systems confined in different geometries, *The European Physical Journal D* 75 (2021) 1–7.
- [37] G. Micca Longo, S. Longo, D. Giordano, Spherically confined H2+: and states, *Physica Scripta* 90 (2) (2015) 025403.
- [38] G. Micca Longo, S. Longo, D. Giordano, Quantum states of confined hydrogen plasma species: Monte Carlo calculations, *Plasma Sources Sci. Technol.* 24 (6) (2015) 065019.
- [39] S. Longo, G. Micca Longo, D. Giordano, Monte Carlo calculation of the potential energy surface for octahedral confined H 2+, *Rendiconti Lincei. Scienze Fisiche e Naturali* 29 (1) (2018) 173–177.
- [40] M.W. Zemansky, *Heat and Thermodynamics*, 5th ed., McGraw-Hill, New York, 1968.
- [41] V.N. Zharkov, *Interior Structure of the Earth and Planets*, Harwood, New York, 1986.
- [42] A. Jayaraman, Diamond anvil cell and high-pressure physical investigations, *Rev. Mod. Phys.* 55 (1) (1983) 65.
- [43] T. Guillot, Interiors of giant planets inside and outside the solar system, *Science* 286 (5437) (1999) 72–77.
- [44] G. Micca Longo, L. Vialletto, P. Diomede, S. Longo, V. Laporta, Plasma modeling and prebiotic chemistry: A review of the state-of-the-art and perspectives, *Molecules* 26 (12) (2021) 3663.