

Classification of Shapes and Deformations of Large Systems by Invariant Coordinates

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Abstract. The use of hyperspherical coordinates is widespread in reactive scattering studies, allowing for a symmetric representation of the quantum dynamics of reactive processes. Indeed, among the variants of hyperspherical coordinates, the so called "symmetric" ones are "democratic" with respect to the asymptotic channels and so are the corresponding basis sets, since basis functions can be symmetrized with respect to particle exchange, acting on just a reduced subset of coordinates. Applications to scattering problems are limited to few-atom systems, due to computational cost. An extension of the representation to many-body classical dynamics is possible and has been proposed in a series of papers, where different aspects have been investigated. Here we recall the possibility of defining shape coordinates invariant with respect to the remaining degrees of freedom, which are suitable for systematic classification of structures of clusters and large biomolecules. The definition of shape parameters and to provide examples of their application are the purposes of the present paper.

Keywords: Hyperspherical coordinates · Intermolecular interactions · Atomic clusters · Global minimum · Isomers · Shape coordinates

1 Introduction

The hyperspherical approach to molecular dynamics is well suited for quantum reactive scattering calculations and has been extensively adopted during the last decades, when efforts have been dedicated to the definition of sets of hyperspherical functions [1–3] for three and four-body collision dynamics (see e.g. [4–9]). The Hamiltonian in "symmetric" hyperspherical coordinates is invariant with respect to the possible product arrangements, typical of multi-channel processes, and for such reason the hyperspherical one is largely preferable with respect to other approaches. A further benefit of the use of hyperspherical coordinates is that the hyperspherical basis functions, conveniently chosen, can be used to represent the intermolecular and intramolecular interactions [10–36].

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The use of hyperspherical method is not restricted to quantum dynamics, where it is limited to systems of three or four atoms, but can be extended to classical dynamics, to simulate large molecules and atomic and molecular clusters, liquids and solids, taking advantage of the reduced computational cost of classical trajectories (see e.g. [37]).

The hyperspherical coordinates separate the degrees of freedom into homogeneous sets of variables, each contributing separately to the kinetic energy, and these are shape deformation coordinates, ordinary rotations and kinematic rotations angles [6,38–42]. The corresponding kinetic energy terms are defined in the classical mechanics framework by the hyperangular momenta appearing in the Hamilton function, which, apart from some purely quantum extra-terms, not present in classical mechanics, can be put into correspondence with the quantum Hamiltonian operator. Although classical equations of motion could in principle be obtained and integrated in hyperspherical form, integration in Cartesian coordinates is much more convenient. A procedure based on matrix transformations of the set of position vectors has been developed, which allows for the evaluation of the energy terms appearing in the Hyperspherical Hamilton function as a function of time [6,39].

It is relevant for us that the hyperspherical separation scheme of the degrees of freedom introduce ordinary rotations and rotations in the kinematic space, under the action of which the global shape of the system in the three-dimensional physical space is invariant, meaning that the remaining three degrees of freedom must be themselves invariant with respect to both kinds of rotations. This "invariance" approach to classical dynamics of molecules and clusters has been investigated in previous papers [38,43–48].

Here, we consider the use of invariant hyperspherical shape parameters for the classification of local and global minimum energy structures of atomic and molecular clusters.

2 Theoretical Background

The hyperspherical coordinates are defined for an N-particle system starting from the corresponding set of $N-1$ Jacobi vectors $\mathbf{Q}_\alpha$, with $\alpha = 1, \cdots, N-1$, a combinations of the radial vectors of the particles in the center of mass reference frame, the latter denoted by $\mathbf{r}_\alpha$ [38]. A "canonical" sequential generation of such vectors is as follows: take the vector which connects particles 1 and 2, then the one connecting the center of mass of the pair to the third particle, and so on, up to the $(N-1)$th vector, which connects the center of mass of the first $N-1$ particles to the Nth particle. The coefficients of the combination depends on the particle masses, see Sect. 2.1 for details. The next step consists in the definition of an hyperradius ρ as the modulus of a vector of dimension $3N-3$, spanning the configuration space of the system. The Cartesian components of the hyperradial vector, is given by the ordered sequence of the Jacobi vector components, which can be expressed as a function of the hyperradius itself and $3N-4$ "hyperangles", which define the hyperspherical coordinate system. There are in principle many

alternatives for the choice of the a angular variables, but the most interesting for us is the one who leads to the so called Symmetric hyperspherical representation. In algebraic terms, this is the result of a matrix transformation, the *singular value decomposition*, operating on a properly constructed position matrix. The procedure to generate hyperspherical coordinates is described in the following section.

2.1 Hyperspherical Coordinates for Atomic and Molecular Aggregates

An appropriate mathematical tool for the representation of N-center systems is the *singular value decomposition* [49], a matrix decomposition theorem that can be applied to any given set of N vectors arranged column-wise to form a $3 \times N$ position matrix.

Let us suppose we have a collection of $N \geq 2$ particles with masses $m_1, \cdots, m_N$ and positions identified by a set of radii vectors in the center of mass reference frame, $\mathbf{r_1}, \cdots, \mathbf{r_N}$. Mass *scaled* radii vectors $\mathbf{q}_\alpha = (m_\alpha/M)^{1/2}\mathbf{r}_\alpha$ $(1 \leq \alpha \leq N)$, can be obtained, where $M = \sum_\alpha^N m_\alpha$ is the total mass of the system.

A $3 \times N$ position matrix denoted by Z containing column-wise the components of the mass scaled vectors, can be generated, as follows:

$$Z = \begin{pmatrix} q_{1,1} & q_{1,2} & \cdots & q_{1,N} \\ q_{2,1} & q_{2,2} & \cdots & q_{2,N} \\ q_{3,1} & q_{3,2} & \cdots & q_{3,N} \end{pmatrix}. \tag{1}$$

The coordinate frame can be rotated, by the action of an orthogonal matrix R^t (transpose of a matrix $R \in O(3)$) on the position matrix Z by left-multiplication. An orthogonal matrix $K \in O(N)$ acting in the position matrix by right-multiplication instead rotates the coordinate frame in the so called *kinematic space* [5,39], $Z' = ZK$.

It is possible to identify a subset of K matrices having the following form (see last column):

$$K = \begin{pmatrix} k_{1,1} & k_{1,2} & \cdots & (m_1/M)^{1/2} \\ k_{2,1} & k_{2,2} & \cdots & (m_2/M)^{1/2} \\ \cdots & \cdots & \cdots & \cdots \\ k_{N,1} & k_{N,2} & \cdots & (m_N/M)^{1/2} \end{pmatrix} \tag{2}$$

and its application to the Z matrix generates a subset of all the possible Cartesian frames. Remarkably, the elements of the last column of such Z matrices are identically zero, due to the relation $\sum_\alpha^N m_\alpha^{1/2}\mathbf{q}_\alpha = 0$, valid for the mass scaled vectors and that has the physical meaning of separating the motion of the center of mass, so reducing the number of necessary degrees of freedom to $3N - 3$. This smaller matrix Z is called *reduced position matrix*.

The sets of $(N-1)$ Jacobi and related vectors invariably form reduced matrices. The Jacobi vectors are obtained as a linear combinations of the N Cartesian particle position vectors, with coefficients being a function of the particle masses [50,51]. Different Jacobi vector sets are possible, corresponding to the different particle coupling schemes, a representation of the reactive channels of the system; the sets are smoothly connected by coordinate transformation in the kinematic space.

The *singular value decomposition* theorem applied to the $3\times n$ position matrix Z (where $n = N$ or $n = N-1$) gives a product of three matrices:

$$Z = R\Xi K^t \tag{3}$$

where $R \in O(3)$ and $K \in O(n)$ are 3×3 and $3 \times n$ orthogonal matrices, respectively. The elements of the $3 \times n$ matrix Ξ are zeroes, with the possible exception of the diagonal entries, $\Xi_{11} = \xi_1, \Xi_{22} = \xi_2, \Xi_{33} = \xi_3$, which are subjected to the inequality $\xi_1 \geq \xi_2 \geq \xi_3 \geq 0$.

The values $\xi_i, (i = 1, 2, 3)$ are called the *singular values* of the matrix Z and are uniquely determined, although the factors R and K in Eq. 3 are not. If $N \leq 3$ and Z is the full $3\times N$ position matrix, then the smallest singular value ξ_3 is necessarily zero. The singular values are connected to the hyperradius as follows [38,39]:

$$\xi_1^2 + \xi_2^2 + \xi_3^2 = \rho^2. \tag{4}$$

The ξ's are invariant under both ordinary rotations in the physical space and kinematic rotations [5,6,39,52], a property that can be exploited in molecular dynamics [38,53–56] and in the study of the minimum energy structures of N-particle aggregates.

In the case $n = N - 1 = 3$, the matrix Z represent four particles or four center systems. In this special case, the two matrices R and K cannot be chosen to be *special orthogonal* ($R \in SO(3)$ and $K \in SO(n)$), but are required to be just orthogonal matrices ($O(3)$). Under such circumstances, if the determinant of Z is lower than zero, its sign depends on the sign of the product of the ξ's, and so one has $\xi_3 \leq 0$. This fact is directly connected to the mirror image and chirality sign of the system [43,57,58].

The previous matrix transformation has the effect of partitioning the $3N-3$ degrees of freedom into three distinct sets of coordinates: three angles, parametrizing the rotation matrix R and accounting for spatial rotations, $3N-9$ angles, parametrizing the rotation matrix K, accounting for rotations in the kinematic space, and 3 ξ's, the invariant quantities which are related to the hyperradius, being the only quantities with units of length.

2.2 Hyperradius and Invariant Deformation Indexes

The singular values (ξ_1, ξ_2, ξ_3) are invariant under the action of kinematic and ordinary rotations [59] and are related to the moments of inertia of the system, as follows:

$$\begin{aligned} \frac{I_1}{M} &= \xi_2^2 + \xi_3^2 \\ \frac{I_2}{M} &= \xi_1^2 + \xi_3^2 \\ \frac{I_3}{M} &= \xi_1^2 + \xi_2^2 \end{aligned} \tag{5}$$

where I_1, I_2 and I_3 are the moments of inertia in the principal axis reference frame. From Eq. 4 one obtains:

$$I_1 + I_2 + I_3 = 2M\rho^2. \tag{6}$$

It is clear how the relative values of the ξ's determine whether the system is an asymmetric, symmetric or a spherical rotor. Spherical top configurations are those for which $\xi_1 = \xi_2 = \xi_3$, prolate tops those for which $\xi_3 = \xi_2 < \xi_1$, while oblate tops occur when $\xi_1 = \xi_2 > \xi_3$.

It is convenient to parametrize the ξ's in terms of the hyperradius and two angles θ and ϕ as follows:

$$\begin{aligned} \xi_1 &= \rho \sin\theta \cos\phi \\ \xi_2 &= \rho \sin\theta \sin\phi \\ \xi_2 &= \rho \cos\theta \end{aligned} \tag{7}$$

Parameters measuring the deviation from the spherical top shapes, can be introduced by two following *deformation indexes* [38]:

$$\xi_+ = \frac{\xi_2^2 - \xi_3^2}{\rho^2}, \;\; \xi_+ \geq 0 \tag{8}$$

which is zero for prolate top configurations, and

$$\xi_- = \frac{\xi_2^2 - \xi_1^2}{\rho^2}, \;\; \xi_- \leq 0 \tag{9}$$

which is zero for oblate top configurations. By definition, when both indexes are zero, one has a spherical rotor.

2.3 Deformation Indexes of Atomic and Molecular Clusters

Being the deformation indexes rotationally invariant (in the sense illustrated in the previous sections) they can naturally be used to classify global structures of large molecular systems, looking for patterns and regularities in the global an local minimum energy structures. As an example of application, we consider

sets of global and local minima of simple Lennard-Jones clusters. To calculate the indexes, one needs the values of the invariant ξ's for each cluster structure. A direct way to get them is to use the following relation coming from Eq. 3:

$$ZZ^t = R\Xi\Xi^t R^t \tag{10}$$

where the product $\Xi\Xi^t$ is 3×3 square diagonal matrix, whose entries are the squares of the ξ's. The diagonal entries are just the eigenvalues of the matrix product ZZ^t involving the position matrix. Using the Cartesian components of the mass scaled atomic position vectors (see Sect. 2.1), one has to calculate the ZZ^t matrix and diagonalize it, numerically, or by using the well known Cardano's formula for the characteristic equation [38].

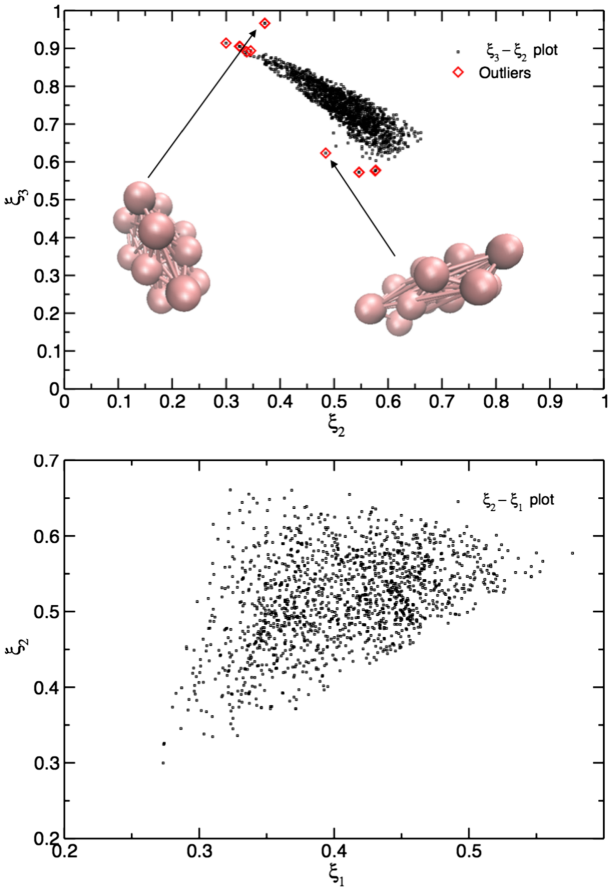

Fig. 1. Two-dimensional plots of the ξ_i, $i = 1, 2, 3$ invariants for the entire set of global and local minima of a 13-atom Lennard-Jones (LJ) 12-6 cluster. (See Ref. [38] for a 12-atom cluster). Structures have been obtained from the database [60]

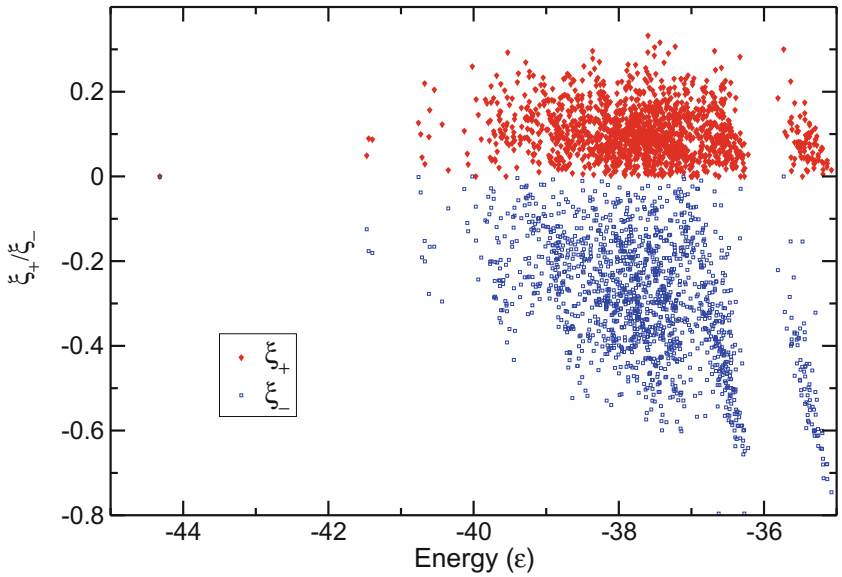

Fig. 2. Plot of the ξ_+ and ξ_+ deformation indexes as a function of energy, for the global and minimum energy structures of a 13-atom Lennard-Jones cluster.

The series of local minimum structures, are those freely available at the Cambridge Cluster Database [60], for the 13-atom Lennard-Jones cluster. In Fig. 1, the invariant ξ's of Sect. 2.2 for the LJ cluster minima are reported in two panels where ξ_3-ξ_2 plots (upper panel) and ξ_2-ξ_3 plots (lower panels) are represented. Note that the allowed values are restricted to a partial subspace. Some outliers, corresponding to very deformed structure are indicated.

In Fig. 2 the deformation indexes ξ_+ and ξ_- are shown for the same minimum energy structures, as a function of energy in terms of the Lennard-Jones well dept ϵ. The trend shows marked oscillations, interrupted by the occurrence of spherical top configurations, where strong deviations from the spherical top configuration occur. Some energy gaps can be noticed, where no minima are present.

3 Conclusions

In this paper we outlined some aspects of the hyperspherical coordinate approach to structure and dynamics, that can be applied in a classical mechanics framework to large molecules and clusters. It has been shown the possible use of rotationally invariant quantities and deformation indexes to classify structures and identify outlying geometries, which makes hyperspherical invariants a perspective tool for systematic classification of minimum energy structures of clusters and biomolecules.

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References

1. Zhao, B., Guo, H.: State-to-state quantum reactive scattering in four-atom systems. WIREs Comput. Mol. Sci. **7**, e1301 (2017)
2. Skouteris, D., Castillo, J., Manolopoulos, D.E.: Abc: a quantum reactive scattering program. Comput. Phys. Comm. **133**, 128–135 (2000)
3. Lepetit, B., Launay, J.M.: Quantum-mechanical study of the reaction $He+H_2^+ \rightarrow HeH^+ + H$ with hyperspherical coordinates. J. Chem. Phys. **95**, 5159–5168 (1991)
4. Aquilanti, V., Beddoni, A., Cavalli, S., Lombardi, A., Littlejohn, R.: Collective hyperspherical coordinates for polyatomic molecules and clusters. Mol. Phys. **98**(21), 1763–1770 (2000)
5. Aquilanti, V., Beddoni, A., Lombardi, A., Littlejohn, R.: Hyperspherical harmonics for polyatomic systems: basis set for kinematic rotations. Int. J. Quantum Chem. **89**(4), 277–291 (2002)
6. Aquilanti, V., Lombardi, A., Littlejohn, R.: Hyperspherical harmonics for polyatomic systems: basis set for collective motions. Theor. Chem. Acc. **111**(2–6), 400–406 (2004)
7. Kuppermann, A.: Quantum reaction dynamics and hyperspherical harmonics. Isr. J. Chem. **43**, 229 (2003)
8. De Fazio, D., Cavalli, S., Aquilanti, V.: Benchmark quantum mechanical calculations of vibrationally resolved cross sections and rate constants on ab initio potential energy surfaces for the F + HD reaction: comparisons with experiments. J. Phys. Chem. A **120**, 5288–5299 (2016)
9. Aquilanti, V., Cavalli, S.: The quantum-mechanical hamiltonian for tetraatomic systems insymmetric hyperspherical coordinates. J. Chem. Soc., Faraday Trans. **93**, 801–809 (1997)
10. Lombardi, A., Laganà, A., Pirani, F., Palazzetti, F., Faginas-Lago, N.: Carbon oxides in gas flows and earth and planetary atmospheres: state-to-state simulations of energy transfer and dissociation reactions. In: Murgante, B., Misra, S., Carlini, M., Torre, C., Nguyen, H.Q., Taniar, D., Apduhan, B., Gervasi, O. (eds.) Computational Science and Its Applications - ICCSA 2013. Lecture Notes in Computer Science, vol. 7972, pp. 17–31. Springer, Berlin Heidelberg (2013). https://doi.org/10.1007/978-3-642-39643-4_2
11. Lago, N.F., Albertí, M., Laganà, A., Lombardi, A.: Water $(H_2O)_m$ or benzene $(C_6H_6)_n$ aggregates to solvate the K^+. In: Murgante, B., et al. (eds.) ICCSA 2013. LNCS, vol. 7971, pp. 1–15. Springer, Heidelberg (2013). https://doi.org/10.1007/978-3-642-39637-3_1

12. Faginas-Lago, N., Albertí, M., Costantini, A., Laganá, A., Lombardi, A., Pacifici, L.: An innovative synergistic grid approach to the computational study of protein aggregation mechanisms. J. Mol. Model. **20**(7), 2226 (2014)
13. Faginas-Lago, N., Yeni, D., Huarte, F., Alcamì, M., Martin, F.: Adsorption of hydrogen molecules on carbon nanotubes using quantum chemistry and molecular dynamics. J. Phys. Chem. A **120**, 6451–6458 (2016)
14. Faginas-Lago, N., Lombardi, A., Albertí, M., Grossi, G.: Accurate analytic intermolecular potential for the simulation of Na^+ and K^+ ion hydration in liquid water. J. Mol. Liq. **204**, 192–197 (2015)
15. Albertí, M., Faginas Lago, N.: Competitive solvation of K^+ by C_6H_6 and H_2O in the K^+-$(C_6h_6)_n$-$(H_2O)_m$ (n = 1–4; m = 1–6) aggregates. Eur. Phys. J. D **67**, 73 (2013)
16. Albertí, M., Faginas Lago, N.: Ion size influence on the ar solvation shells of M^+-C_6F_6 clusters (m = na, k, rb, cs). J. Phys. Chem. A **116**, 3094–3102 (2012)
17. Albertí, M., Faginas Lago, N., Pirani, F.: Ar solvation shells in K^+-HFBz: From cluster rearrangement to solvation dynamics. J. Phys. Chem. A **115**, 10871–10879 (2011)
18. Lago, N.F., Albertí, M., Laganà, A., Lombardi, A., Pacifici, L., Costantini, A.: The molecular stirrer catalytic effect in methane ice formation. In: Murgante, B., et al. (eds.) ICCSA 2014. LNCS, vol. 8579, pp. 585–600. Springer, Cham (2014). https://doi.org/10.1007/978-3-319-09144-0_40
19. Faginas-Lago, N., Huarte Larrañaga, F., Albertí, M.: On the suitability of the ilj function to match different formulations of the electrostatic potential for water-water interactions. Eur. Phys. J. D **55**(1), 75 (2009)
20. Bartolomei, M., Pirani, F., Laganà, A., Lombardi, A.: A full dimensional grid empowered simulation of the CO_2+ CO_2 processes. J. Comp. Chem. **33**, 1806 (2012)
21. Lombardi, A., Faginas-Lago, N., Laganà, A., Pirani, F., Falcinelli, S.: A bond-bond portable approach to intermolecular interactions: Simulations for n-methylacetamide and carbon dioxide dimers. In: Murgante, B., et al. (eds.) Computational Science and Its Applications - ICCSA 2012. Lecture Notes in Computer Science, vol. 7333, pp. 387–400. Springer, Berlin Heidelberg (2012). https://doi.org/10.1007/978-3-642-31125-3_30
22. Albertí, M., Faginas-Lago, N., Laganà, A., Pirani, F.: A portable intermolecular potential for molecular dynamics studies of nma-nma and nma-H_2O aggregates. Phys. Chem. Chem. Phys. **13**(18), 8422–8432 (2011)
23. Albertí, M., Faginas-Lago, N., Pirani, F.: Benzene water interaction: from gaseous dimers to solvated aggregates. Chem. Phys. **399**, 232 (2012)
24. Falcinelli, S., Rosi, M., Candori, P., Vecchiocattivi, F., Bartocci, A., Lombardi, A., Faginas-Lago, N., Pirani, F.: Modeling the intermolecular interactions and characterization of the dynamics of collisional autoionization processes. In: Murgante, B., et al. (eds.) Computational Science and Its Applications - ICCSA 2013. Lecture Notes in Computer Science, vol. 7971, pp. 69–83. Springer, Berlin Heidelberg (2013). https://doi.org/10.1007/978-3-642-39637-3_6
25. Lombardi, A., Faginas-Lago, N., Pacifici, L., Costantini, A.: Modeling of energy transfer from vibrationally excited CO_2 molecules: cross sections and probabilities for kinetic modeling of atmospheres, flows, and plasmas. J. Phys. Chem. A **117**(45), 11430–11440 (2013)

26. Lombardi, A., Pirani, F., Laganà, A., Bartolomei, M.: Energy transfer dynamics and kinetics of elementary processes (promoted) by gas-phase CO_2-N_2 collisions: selectivity control by the anisotropy of the interaction. J. Comp. Chem. **37**, 1463–1475 (2016)
27. Pacifici, L., Verdicchio, M., Faginas-Lago, N., Lombardi, A., Costantini, A.: A high-level ab initio study of the n2 + n2 reaction channel. J. Comput. Chem. **34**(31), 2668–2676 (2013)
28. Lombardi, A., Faginas-Lago, N., Pacifici, L., Grossi, G.: Energy transfer upon collision of selectively excited CO_2 molecules: state-to-state cross sections and probabilities for modeling of atmospheres and gaseous flows. J. Chem. Phys. **143**, 034307 (2015)
29. Celiberto, R., et al.: Atomic and molecular data for spacecraft re-entry plasmas. Plasma Sources Sci. Technol. **25**(3), 033004 (2016)
30. Faginas-Lago, N., Lombardi, A., Albertí, M.: Aqueous n-methylacetamide: new analytic potentials and a molecular dynamics study. J. Mol. Liq. **224**, 792–800 (2016)
31. Palazzetti, F., Munusamy, E., Lombardi, A., Grossi, G., Aquilanti, V.: Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. Int. J. Quantum Chem. **111**(2), 318–332 (2011)
32. Lombardi, A., Palazzetti, F.: A comparison of interatomic potentials for rare gas nanoaggregates. J. Mol. Struc-THEOCHEM **852**(1–3), 22–29 (2008)
33. Barreto, P.R., Albernaz, A.F., Palazzetti, F., Lombardi, A., Grossi, G., Aquilanti, V.: Hyperspherical representation of potential energy surfaces: intermolecular interactions in tetra-atomic and penta-atomic systems. Phys. Scr. **84**(2), 028111 (2011)
34. Barreto, P.R., et al.: Potential energy surfaces for interactions of H^2O with H_2, N_2 and O_2: a hyperspherical harmonics representation, and a minimal model for the H_2O-rare-gas-atom systems. Comput. Theor. Chem. **990**, 53–61 (2012)
35. Lombardi, A., Pirani, F., Bartolomei, M., Coletti, C., Laganà, A.: A full dimensional potential energy function and the calculation of the state-specific properties of the CO+ N_2 inelastic processes within an Open Molecular Science Cloud perspective. Front. Chem. **7**, 309 (2019)
36. Faginas Lago, N., Lombardi, A., Vekeman, J., Rosi, M., et al.: Molecular dynamics of CH_4/N_2 mixtures on a flexible graphene layer: adsorption and selectivity case study. Front. Chem. **7**, 386 (2019)
37. Nakamura, M., et al.: Dynamical, spectroscopic and computational imaging of bond breaking in photodissociation: roaming and role of conical intersections. Faraday Discuss. **177**, 77–98 (2015)
38. Aquilanti, V., Lombardi, A., Yurtsever, E.: Global view of classical clusters: the hyperspherical approach to structure and dynamics. Phys. Chem. Chem. Phys. **4**(20), 5040–5051 (2002)
39. Sevryuk, M.B., Lombardi, A., Aquilanti, V.: Hyperangular momenta and energy partitions in multidimensional many-particle classical mechanics: the invariance approach to cluster dynamics. Phys. Rev. A **72**(3), 033201 (2005)
40. Castro Palacio, J., Velazquez Abad, L., Lombardi, A., Aquilanti, V., Rubayo Soneira, J.: Normal and hyperspherical mode analysis of no-doped kr crystals upon rydberg excitation of the impurity. J. Chem. Phys. **126**(17), 174701 (2007)
41. Lombardi, A., Palazzetti, F., Aquilanti, V.: Molecular dynamics of chiral molecules in hyperspherical coordinates. In: Misra, S., et al. (eds.) ICCSA 2019. LNCS, vol. 11624, pp. 413–427. Springer, Cham (2019). https://doi.org/10.1007/978-3-030-24311-1_30

42. Lombardi, A., Palazzetti, F., Sevryuk, M.B.: Hyperspherical coordinates and energy partitions for reactive processes and clusters. In: AIP Conference Proceedings. Volume 2186, p. 030014. AIP Publishing LLC (2019)
43. Lombardi, A., Palazzetti, F.: Chirality in molecular collision dynamics. J. Condens. Matter Phys. **30**(6), 063003 (2018)
44. Lombardi, A., Palazzetti, F., Peroncelli, L., Grossi, G., Aquilanti, V., Sevryuk, M.: Few-body quantum and many-body classical hyperspherical approaches to reactions and to cluster dynamics. Theor. Chem. Acc. **117**(5–6), 709–721 (2007)
45. Aquilanti, V., Grossi, G., Lombardi, A., Maciel, G.S., Palazzetti, F.: Aligned molecular collisions and a stereodynamical mechanism for selective chirality. Rend. Fis. Acc. Lincei **22**, 125–135 (2011)
46. Lombardi, A., Faginas-Lago, N., Aquilanti, V.: The invariance approach to structure and dynamics: classical hyperspherical coordinates. In: Misra, S., et al. (eds.) ICCSA 2019. LNCS, vol. 11624, pp. 428–438. Springer, Cham (2019). https://doi.org/10.1007/978-3-030-24311-1_31
47. Caglioti, C., Dos Santos, R.F., Lombardi, A., Palazzetti, F., Aquilanti, V.: Screens displaying structural properties of aminoacids in polypeptide chains: alanine as a case study. In: Misra, S., et al. (eds.) ICCSA 2019. LNCS, vol. 11624, pp. 439–449. Springer, Cham (2019). https://doi.org/10.1007/978-3-030-24311-1_32
48. Caglioti, C., Ferreira, R.d.S., Palazzetti, F., Lombardi, A., Aquilanti, V.: Screen representation of structural properties of alanine in polypeptide chains. In: AIP Conference Proceedings. Volume 2186, p. 030015, AIP Publishing LLC (2019)
49. Horn, R.A., Johnson, C.R.: Matrix Analysis, 2nd edn. University Press, Cambridge (1990)
50. Gatti, F., Lung, C.: Vector parametrization of the n-atom problem in quantum mechanics. i. jacobi vectors. J. Chem. Phys. **108**(21), 8804–8820 (1998)
51. Aquilanti, V., Lombardi, A., Yurtsever, E.: Global view of classical clusters: the hyperspherical approach to structure and dynamics. Phys. Chem. Chem. Phys. **4**, 5040–5051 (2002)
52. Aquilanti, V., Lombardi, A., Sevryuk, M.B.: Phase-space invariants for aggregates of particles: hyperangular momenta and partitions of the classical kinetic energy. J. Chem. Phys. **121**, 5579 (2004)
53. Aquilanti, V., Carmona Novillo, E., Garcia, E., Lombardi, A., Sevryuk, M.B., Yurtsever, E.: Invariant energy partitions in chemical reactions and cluster dynamics simulations. Comput. Mat. Sci. **35**, 187–191 (2006)
54. Aquilanti, V., Lombardi, A., Sevryuk, M.B., Yurtsever, E.: Phase-space invariants as indicators of the critical behavior of nanoaggregates. Phys. Rev. Lett. **93**, 113402 (2004)
55. Calvo, F., Gadea, X., Lombardi, A., Aquilanti, V.: Isomerization dynamics and thermodynamics of ionic argon clusters. J. Chem. Phys. **125**, 114307 (2006)
56. Lombardi, A., Aquilanti, V., Yurtsever, E., Sevryuk, M.B.: Specific heats of clusters near a phase transition: energy partitions among internal modes. Chem. Phys. Lett. **30**, 424–428 (2006)
57. Lombardi, A., Maciel, G.S., Palazzetti, F., Grossi, G., Aquilanti, V.: Alignment and chirality in gaseous flows. J. Vacuum Soc. Japan **53**(11), 645–653 (2010)
58. Palazzetti, F., et al.: Aligned molecules: chirality discrimination in photodissociation and in molecular dynamics. Rendiconti Lincei **24**(3), 299–308 (2013)
59. Littlejohn, R.G., Mitchell, A., Aquilanti, V.: Quantum dynamics of kinematic invariants in tetra-and polyatomic systems. Phys. Chem. Chem. Phys. **1**, 1259–1264 (1999)
60. Wales, D.G., et al.: The Cambridge Cluster Database (2001)