Ab initio DFT simulation of electronic and magnetic properties of Ti_{n+1} and FeTi_{n} clusters

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Abstract
We report a computational investigation of the electronic and magnetic properties of neutral Ti_{n+1} and FeTi_{n} (n = 1–10) clusters using ab initio calculations based on density functional theory (DFT) within the generalized gradient approximation (GGA). The best structures for Ti_{n+1} and FeTi_{n} clusters are planar for size n ≤ 5, while from n = 5, they showed a compact three-dimensional cage structure. For the best structures of the FeTi_{n} clusters, the Fe atoms favor the peripheral position with the highest coordination with the neighboring Ti atoms. The evolution as a function of the size of the average binding energies (Eb/atom) and HOMO–LUMO gaps of Ti_{n+1} and FeTi_{n} (n = 1–10) clusters are studied. The stability results show that the Ti_{n+1} clusters have relatively higher stability than the FeTi_{n} cluster with the same size. In addition, the vertical ionization potentials and electron affinities, chemical hardness, and atomic magnetic moment of Ti_{n+1} and FeTi_{n} (n = 1–10) clusters are also investigated.

Keywords Structural properties · Electronic properties · Magnetic properties · DFT-GGA · Clusters · Fe-Ti

Introduction
During the last 4 decades, the semiconductor and transition metal clusters intensively studied because of their specific properties and their great potential use in optoelectronic materials and other nanotechnology areas. The properties of titanium clusters have been investigated because they are interesting for the fine processing and the synthesis of novel materials and the exploration of possibilities of finding novel species and phenomena. Due to the particularity of their properties, the titanium material is applied in many fields especially in medical and different industrial processes. In the literature data, less attention has been allowed to the small titanium clusters. In order to explore and understand the structural, electronic, and magnetic behavior of the pure and doped titanium clusters, different authors have recently carried out many experimental and theoretical works.

A number of theoretical [1–9] and experimental [10–14] studies about pure titanium clusters have been reported. They have drawn much attention for their numerous applications in the nano-electronics area [6–8]. In addition, the doping Ti_{n} clusters with transition metal atom have been often used to change the chemical and physical properties of the small clusters [6–9, 12, 15–19]. In experimental studies, Lian et al. [10] used the collision-induced dissociation for Ti_{n}^{+} (n = 2–22) by using a guided beam mass spectrometer. They found that the evolution of the dissociation energy with the size show local important peaks at n = 7, 13, and 19.

Sakurai et al. [11] using a TOF mass spectrometry of Ti_{n} clusters with up to 30 atoms found that Ti_{7}, Ti_{13}, Ti_{15}, Ti_{19}, and Ti_{25} were the magic numbers. With anion photoelectron spectra, Wu et al. [13] show that the 3d band appears at n = 8 then widens and evolves towards the bulk band in the charged Ti_{n}^{−} (n = 3–65) clusters. Using resonant tow-photon ionization technique, Doverstål et al. [14] studied Ti dimer and found a bond length as 1.9429 ± 0.0013 Å. Neukermans et al. [20, 21], basing on the photo-fragmentation experiments, investigated the stability of Au_{n}X^{+} clusters doped with a 3d atoms from Sc to Ni and Au_{n}X_{m} clusters (X = Sc, Ti, Cr, Fe). Kim et al. [22] studied nanoparticles of Ti-Cr using the electrical wire explosion of electrode-posted metal wires. Koyasu et al. [23] proved experimentally by using...
mass and photoelectron spectroscopies the high stability of MSi_{16} clusters, while Furuse et al. [24] studied the MSi_{16}^{-}, MGe_{16}^{-}, MSi_{16}^{-}, and MPi_{16}^{-} by experimental and theoretical characterization, and they confirmed the exceptional stability for MSi_{16}.

In the theoretical aspect, Anderson [25] investigates with very early Hückel molecular orbital calculations the properties of Ti_{2-6} clusters. Wei et al. [26], by using DFT and LSDA approach, investigated the properties of Ti_{n} (n = 2–10) clusters. They found that Ti, with good stability is a magic number. Zhao et al. [3] studied the properties of Ti_{n} (n = 2–14, 19, and 55) by using the plane wave ultra-soft pseudopotential method and GGA approach. They found a pentagonal growth models for the clusters and a rapid convergence towards bulk bands for electron density of state. Using GGA, Castro [5] investigated the properties of small Ti_{n}^{-} and Ti_{n} (n = 3–8, and 13) clusters. The structures of small Ti_{n} (n = 2–5) were also studied by Duet al. [4], Salazar-Villanueva [27] investigated the structure of Ti_{n} (n = 2–15) clusters, and they identified that they are three magic number clusters n = 7, 13, and 15. Lee et al. [28] studied the stability of titanium clusters taking into account the spin polarization and structural distortion. The magnetic properties of Ti_{n} (n = 2–13) clusters have been studied by Medina et al. [29]. By using genetic algorithm, Lazauskas et al. [30] investigate the potential energy surface (PES) for small Ti_{n} (n = 2–32) clusters. Sun et al. [1] studied by fully self-consistent DFT-based calculation the evolution as a function of the size of the electronic properties of Ti_{n} (n = 2–20). The stabilization mechanism of Ti_{n} clusters with n = 3, 4, 5, 7, 13, 15, and 19 have also investigated by Sun et al. [2]. The same author and their co-workers have also studied the magnetic and structural properties of Ti_{12}M clusters (M = Sc to Zn) [8] and Ti_{n}M, Al_{n} (n = 2–8, 13, x = 0–n) [15], by using the DFT approach. Some other authors are also interested in the properties of titanium clusters such as Ni_{3}Ti_{x} (x + y ≤ 5) [16], Ti_{P} (n = 1–12) [17], Au_{n}Ti (n = 1–9) [18], Ti-Ni clusters [6, 7], Pt_{m}M_{y} (M = Ti, V) [19], and Ga_{n}Ti_{n}^{0} (n = 1–10) [31].

The purpose of this study is to investigate by using the ab initio and DFT approach of the different properties of the small-sized titanium clusters doped by iron atom. In the literature data, to our knowledge, there are no studies on the small neutral and iron-doped titanium clusters until now. In addition, many recent studies have reported the importance of Fe atom in the stabilization of metallic and semiconductor structures and that Ti-Fe alloys have good physical properties [32] and significant photocatalytic properties [33]. Moreover, Fe-Ti alloys are very important in the treatment of pollution by some chemical elements and their ecological damage, such as antimony Sb [34]. Therefore, the geometries, stabilities, electronic, and magnetic properties of Ti_{n} and FeTi_{n} (n = 1–10) clusters will be studied. We hoped that our results will provide powerful guidelines for further studies and would be helpful to understand the effect of the introduction of transition metal impurity on the metallic and semiconducting cages and its properties. The article is organized as follows. In the “Methods” section, we give the theoretical methods and simulation parameters which are used in this study. Presentation and the analysis of the obtained results are presented in the “Results and discussion” section, finally we give the conclusions of this work in the “Conclusion” section.

Methods

In this work, all of the calculations on the geometry optimizations of FeTi_{n} clusters were performed using DFT approach [35] in the generalized gradient approximation (GGA) with the Perdew, Burke, and Ernzerhof (PBE) parameterization [36] for the exchange–correlation term, implemented in the SIESTA package [37]. In order to obtain the best energy structure, a large number of possible initial structures have been considered in geometry optimizations. All geometry optimizations are done with any symmetry constraints. Using the conjugate gradient scheme, the geometries are relaxed without any symmetry constraints. A large supercell with side-length of 40 Å is used to avoid the different interaction between the neighboring systems. The single gamma-point (Γ) was used in the k grid integration. Double zeta basis with polarization functions (DZP) was used for both Fe and Ti species. Self-consistent field electronic calculations are done with a convergence condition of 10^{-4} e.u. of the total energy. For the geometry optimization, the convergence criteria is 10^{-5} eV/Å for the forces. The validation of this current computational was performed by the calculations tests on Ti_{2} and Fe_{2} dimers. The obtained results are given in Table 1. It shows the reliability of current computational method to study the small FeTi_{n} clusters.

Results and discussion

Geometrical structures of pure and Fe-doped Ti_{n} clusters

In the first time, we describe the equilibrium structures of pure titanium clusters. The obtained lowest energy structures and their first close isomers are shown in Fig. 1. Their other physical parameters are given in Table 2. For Ti_{2}, the dimer with D_{2h} symmetry, the obtained bond length Ti–Ti is 2.059 Å which is in good agreement with the previous theoretical and experimental values which are given in Table 1. For the trimer Ti_{3} (a), the ground state isomers are triangular structure with C_{3v} symmetry. The average bond length is obtained to be 2.647 Å and an apex angle of 76.911°. For
The geometries exploration of the ground state isomers reveals that the rhombus pyramid (C4v) with 2.226 eV/atom is the lowest energy structures. The best energy structure for Ti6 is a trigonal antiprism (C2v) with 2.536 eV/atom and average bond length Ti–Ti of 2.784 Å. For Ti7, the caped trigonal antiprism Ti7(a) with C1 symmetry is considered as the most stable structure with 2.622 eV/atom. In the case of Ti8, the regular cubic structure with high symmetry Oh (a) is obtained as the lowest energy structure with average binding energy of 2.554 eV/atom. For Ti9, the lowest energy isomer is a capped cubic structure Ti9(a) with average binding energy of 2.808 eV/atom and C1 symmetry. Bi-capped square antiprism Ti10 (a) with symmetry Cs and binding energy of 2.946 eV/atom is found as the lowest energy isomers for n = 10. Likewise spherical compact structure with one core atom, bending energy of 3.069 eV/atom and C1 symmetry obtained as the best structure for Ti11.

For doped FeTi clusters, the most stable structures and their corresponding isomers are shown in Fig. 2. For FeTi dimer, the bond length Fe-Ti is 2.941 Å much larger than their corresponding Ti dimer. As in the case of Ti, the best isomer of FeTi2 is triangular structure with Fe-Ti bond length of 2.887 Å and C2v symmetry. For FeTi3, the lowest energy structure is triangular-based pyramid with binding energy 1.752 eV/atom and C3v symmetry. In the case of FeTi4 cluster, a bi-capped tetrahedron with binding energy of 1.949 eV/atom and C3v for symmetry is found as the best isomer. For FeTi5, the best isomer is a distorted bi-capped tetragonal structure with 2.322 eV/atom and C4v symmetry. In the case of FeTi7, our calculations show that the tri-capped triangular base pyramid structure is the most stable one with Cs symmetry. The Fe atom is located at the surface of the cluster cage and highly coordinated to all of the other Ti atoms in the system. The lowest energy isomer for FeTi7 is by the composition of rectangular and tetragonal bi-capped structures with O4h symmetry and binding energy of 2.576 eV/atom. This structure is only 0.041 eV/atom more stable than their first isomer FeTi7 (b) with D4h symmetry. For FeTi8, the most stable structure is composed by two distorted tetragonal-based pyramid with binding energy of 2.786 eV/atom and high symmetry D2d. The lowest energy isomer for FeTi9 is a-like-spherical compact structure with Fe atom occupied a peripheral position (C1) and binding energy of 2.792 eV/atom. In the case of FeTi10, the lowest energy structure is a Fe centered a bi-capped cubic structure with 2.925 eV/atom and high symmetry D4h. The centered position and the high coordination number of Fe atom can be the origin of the good stability of this structure. As we see from Table 2 to Table 3, the average bond length of both Ti+n+1 and FeTi n (n = 1–10) show an increasing tendency as the cluster size increases. In addition, in the most of the best structure of FeTi clusters, the Fe atom occupies the highest coordinated site in the clusters, and this behavior increases as the size of cluster increases. These two geometrical parameters can have direct consequences on hybridization between Fe and Ti atoms. It turns out a considerable changing of the clusters electronic and magnetic properties.

### Table 1 Comparison of our calculated bond length of Ti2 and Fe2 with previous experimental and theoretical values

| Dimer   | This work | Theoretical value | Experimental value |
|---------|-----------|-------------------|--------------------|
| Ti2     | 2.059     | 1.98a, 1.971b, 1.969c, 1.951d, 1.954e, 1.944f | 1.97g, 1.945h, 1.943i |
| Fe2     | 2.126j   | 2.22k, 2.15l, 2.10k, 2.04m, 2.003m          | 2.020±0.2n, 1.87o    |

- a From Ref [29]
- b From Ref [15]
- c From Ref [27]
- d From Ref [8]
- e From Ref [1]
- f From Ref [35]
- g From Ref [36]
- h From Ref [14]
- i From Ref [37]
- j From Ref [38]
- k From Ref [39]
- l From Ref [40]
- m From Ref [41]
- n From Ref [42]
- o From Ref [43]
difference in energy between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO)), the vertical ionization potential (VIP), and the vertical electron affinity (VEA).

The averaged binding energy (Eb/atom) is useful for quantity to study the stability of small clusters. This parameter can be calculated for Ti_{n+1} and FeTi_{n} as follows:

\[ E_b[Ti_{n+1}] = \frac{[n + 1]E(Ti) - E(Ti_{(n+1)})]}{(n + 1)}, \]  
\[ E_b[FeTi_{n}] = \frac{[E(Fe) + nE(Ti)] - E(FeTi_{n})}{(n + 1)}, \]  

where \( E_b(Ti_{n+1}) \) and \( E_b(FeTi_{n}) \) represent, respectively, the total energy of Ti_{n+1} and FeTi_{n} clusters, and E(Ti) and E(Fe) are the energies of Ti and Fe, respectively.

Fig. 1 Optimized geometries of the lowest-energy structures with their isomers and the point group symmetry for Ti_{n+1} (\( n = 1–10 \))
E(Fe) are the single energies for free Ti and Fe atoms. The obtained values of binding energies for two systems are given in Tables 2 and 3. Their evolutions as a function of the size for the most stable clusters of each size are plotted in Fig. 3. We note the monotonically increasing of binding energy with the increasing of cluster size, which means that these clusters will get energy during their growth. Since, the overall stability (binding energy) is supposed to increase and reach the bulk value of titanium, which is experimentally reported to be 4.85 eV [38], where a cluster requires up a very large number of atoms [39]. We can also see that the binding energy for Ti_{n+1} clusters is larger than those of FeTi_{n}, which means that the doping Fe atom does not enhance the stability of host Ti_{n} clusters at small size.

However, we observe, for n = 7 and n = 8, very close equal values of the binding energy of FeTi_{n} cluster and those of corresponding pure Ti_{n+1}. We notice local peaks in the curve of Ti_{n+1} at size n = 2 and n = 6 implying that Ti_{3} and Ti_{7} are more stable than their neighbors where Ti_{7} is reported as a magic number in the previous studies [1, 7, 11]. In addition, FeTi_{3}, FeTi_{5}, and FeTi_{8} show high stabilities compared to their other neighboring clusters.

The second-order energy difference (Δ_{2}E) is calculated for the best structures of each size by using:

Δ_{2}E(T_{n+1}) = E(T_{n+2}) + E(T_{n}) - 2E(T_{n+1}),

(3)
where $E$ represents the total energy for corresponding cluster. In cluster sciences, this quantity $\Delta_2 E$ is an interesting quantity that reflects the relative stability of clusters. The systems with positive values are more stable than those with negative values of $\Delta_2 E$. The calculated value of $\Delta_2 E$ for the most stable Ti$_{n+1}$ and FeTi$_n$ clusters are plotted in Fig. 4.

\[
\Delta_2 E(\text{FeTi}_n) = E(\text{FeTi}_{n+1}) + E(\text{FeTi}_{n-1}) - 2E(\text{FeTi}_n),
\]

where $E$ represents the total energy for corresponding cluster. In cluster sciences, this quantity $\Delta_2 E$ is an interesting quantity that reflects the relative stability of clusters. The systems with positive values are more stable than those with negative values of $\Delta_2 E$. The calculated value of $\Delta_2 E$ for the most stable Ti$_{n+1}$ and FeTi$_n$ clusters are plotted in Fig. 4.

We notice the pronounced positive value of $\Delta_2 E$ at Ti$_7$ for pure Ti$_{n+1}$ indicating that this cluster has a special stability what has already well-mentioned at binding energy (Fig. 3). In addition, this number refers to the magic number cluster observed during the experimental studies [10, 11]. Although HOMO–LUMO gap curve shows a dip at this size, meaning the enhanced stability is due to geometric effects instead of electronic effects [1, 40, 41]. As we can see, FeTi$_6$ is...
less stable than Ti_7, but a prominent maximum is found for FeTi_3, Ti_7, and FeTi_8 indicating that they are more stable than the other clusters.

The measurement of the HOMO–LUMO gap, which depends on the eigenvalues of the HOMO and LUMO energy levels, is important to characterize the electronic properties in clusters. Its knowledge is useful to examine the chemical reactivity and the chemical stability of clusters. A large HOMO–LUMO energy gap indicates a weaker chemical reactivity, and high strength required perturbing the electronic structure and bigger HOMO–LUMO gap signifies a higher stability. Clusters with very large gap have a very low chemical reactivity and a high chemical stability [8, 42]. In Fig. 5, the obtained HOMO–LUMO gaps are plotted as a function of cluster size for pure Ti_{n+1} and doped FeTi_{n} (n = 1–11). It is interesting to note that the obtained HOMO–LUMO gaps varies between 0.164 and 0.991 eV for FeTi_{n} clusters and 0.022–0.843 for Ti_{n+1} clusters, which indicate that the metallic behavior can be observed for these two systems. Thus, these clusters can be used in catalytic reactions applications. The behaviors show a general decrease of the HOMO–LUMO gap as the cluster size increase for both Ti_{n+1} and FeTi_{n} clusters. Also, the FeTi_{n} clusters have generally a smallest HOMO–LUMO gap comparing to a pure Ti_{n+1}, indicating that the Fe doping atom weakens the chemical stability and enhances the metallic behavior for the FeTi_{n} clusters. We observe that the clusters FeTi and Ti_{11} have the largest value of HOMO–LUMO gaps suggesting that these clusters have a higher chemical stability and a smaller chemical reactivity than their neighbors.
In cluster physics, VIP and VEA are considered as important measurement that can reflect the chemical stability of the small clusters. The VIP is calculated by the difference in energy between the cationic and neutral clusters with the same geometry of the neutral structure, and the VEA is the energy difference between the neutral and anionic cluster with the same geometry of the neutral structure. In addition, these two parameters are instructive to examine another quantity, which is the global chemical hardness. The higher value of VIP indicates that they need more energy for the
cluster to lose one electron, and the smaller value of VEA indicates that the cluster is more difficult to accept an electron, meanwhile the neutral cluster is high chemically stable.

The VIP and VEA are defined for pure and doped titanium clusters as:

\[
\text{VIP} = E(Ti_{n+1}^+) - E(Ti_{n+1}), \quad (5)
\]
\[
\text{VEA} = E(Ti_{n+1}^-) - E(Ti_{n+1}), \quad (6)
\]
\[
\text{VIP} = E(FeTi_n^+) - E(FeTi_n), \quad (7)
\]
\[
\text{VEA} = E(FeTi_n^-) - E(FeTi_n^-), \quad (8)
\]

\( E \) is the total energy of the considered neutral cluster, while \( E(Ti_{n+1}^+)/E(FeTi_n^+) \) and \( E(Ti_{n+1}^-)/E(FeTi_n^-) \) are, respectively, the total energies of the cationic and anionic clusters. The obtained results of VIP and VEA are given in Tables 2 and 3, plotted, respectively, in Figs. 6 and 7.

As we see from Fig. 6, the VIP increase monotonically for pure titanium clusters and show an oscillating behavior with a trend to increase with increasing size for iron-doped titanium clusters. In addition, the VIP exhibits obvious odd–even oscillations from the size 2 to 7. From Fig. 7, we observe that the VEA increases with the increasing size \( n \) with an obvious increasing from \( n = 6 \). The largest values of VEA are in general observed for the large sized clusters, which mean that we need more energy to add an electron to the systems, indicating the growing of their stability. Among the Ti_{n+1} and FeTi_{n} clusters, FeTi_{6}, FeTi_{9}, and FeTi_{10} show a pronounced peak for VIP and VEA parameters which indicates their high stability compared to the neighboring clusters.

By using the obtained values of VIP and VEA, we investigated the chemical hardness (\( \eta \)) of Ti_{n+1} and FeTi_{n} clusters. Chemical hardness is an important parameter that characterizes the resistance to charge transfer and the stability of clusters. A large value of chemical hardness corresponds to a less reactivity and a higher stability. According to the maximum hardness principles (PMH) [43], the chemical hardness is calculated by:

\[
\eta = \text{VIP} - \text{VEA}, \quad (9)
\]

The calculated values for the most stables structures of both Ti_{n+1} and FeTi_{n} clusters are given in Tables 2 and 3 and shown in Fig. 8. As we can see from the figure, the chemical hardness has a decreasing evolution with the increasing of the size for FeTi_{n} clusters. Except for \( n = 7 \) and 10 the chemical hardness of FeTi_{n} clusters are higher than the pure Ti_{n+1} clusters with the same number of atoms. Through the PMH of chemical hardness, this result indicates that the doped clusters with higher value of chemical hardness are more stable than the corresponding pure clusters. Among the observed values of \( \eta \), a pronounced peak is observed for FeTi_{2} and FeTi_{3} clusters, which indicate their very less chemical reactivity.
Magnetic properties

The magnetic properties of Ti_{n+1} and FeTi_n are studied under the spin-polarized DFT calculations. These magnetic properties are studied by the evaluation of the total spin magnetic moment, which is calculated by the difference between the Mullikan charge populations for the electrons with spin up and the electrons with spin down. The obtained average atomic of spin magnetic moments (SMM) of the two systems are given in Tables 2 and 3 and
presented in Fig. 9. We observe the same variance tendency for both pure $\text{T}i_{n+1}$ and $\text{FeTi}_n$ clusters. The average SSM for the two systems decrease with the increase of the size until $n = 5$ for $\text{FeTi}_n$ and $n = 7$ for $\text{T}i_n$ clusters. From these sizes, the average SSM for the two systems show an increasing tendency with an oscillating behavior with the increasing of the size. As reported in the previous studies, the bulk titanium is nonmagnetic, but the small $\text{T}i_n$ clusters have significant magnetic moment, and it is sensitive to their structures and geometries [7, 17, 18, 26, 29]. The same behavior
is observed in our results. The FeTi dimer with 3.7 µB has the largest average atomic magnetic moment. This is maybe correlated to its linear structure with a long average bond length. For pure Ti_{n+1}, we notice a local peak at \( n = 2 \) and \( 9 \) with 3.3 µB which are the highest in all clusters.

In order to understand the relation between the magnetic behavior and structural properties of Ti_{n+1} and FeTi_{n} clusters, we represent in Fig. 10 the evolution of the average interatomic distances \( a_0(Ti-Ti) \) and \( a_0(Fe-Ti) \) as a function of cluster size. High differences between \( a_0(Ti-Ti) \) and \( a_0(Fe-Ti) \) are observed for very small (\( n \leq 2 \)) and large (\( n \geq 8 \)) size of clusters. For these clusters, large values of total spin magnetic moment are observed. Between \( n = 2 \) and \( n = 8 \), where the difference between the \( a_0(Ti-Ti) \) and \( a_0(Fe-Ti) \) is small, the total spin magnetic moment shows reduced values. This result constitutes a direct relationship between the magnetic and structural properties.

To understand the origin of average SMM of Ti_{n+1} and FeTi_{n} clusters and to evaluate the contribution of different valence orbital (\( s \) and \( d \)) of the Fe and Ti components, we explore the total and partial densities of states for some low energy structures of the two systems. The obtained results for Ti_{3}, Ti_{6}, FeTi_{1}, FeTi_{2}, and FeTi_{4} clusters are shown in Fig. 11. The spin up densities is plotted as positive and the spin down as negative. From this figure, we can clearly see that the 3d states of Ti and Fe atoms play an important contribution in the determination of the magnetic behavior of the Ti_{n} and FeTi_{n} clusters. The 4s states of Ti and Fe atoms contribute little and almost negligible in the FeTi_{n} systems.

**Conclusions**

In this work, we have systematically investigated the properties of small Ti_{n+1} and FeTi_{n} (\( n = 1–10 \)) clusters by using DFT-GGA with PBE parameterization for the exchange–correlation functional calculations. In the doped FeTi_{n} clusters, the Fe atom occupies preferentially the position near or at the surface of the most favorable geometries. The geometrical structures, stabilities, electronic, and magnetic properties of small Ti_{n+1} and FeTi_{n} are calculated and discussed. The geometric optimizations of Ti_{n+1} clusters show that for each cluster size, multiple isomers and new structures in addition to other structures are obtained in the previous studies. The analyses of the binding energies and second-order energies differences show enhanced stability of FeTi_{3}, FeTi_{5}, and FeTi_{8} clusters. From the HOMO–LUMO gaps, we found that the FeTi and Ti_{4} clusters possess a high chemical stability. The average SSM for the two systems depends on the size of FeTi_{n} and \( n = 7 \) for Ti_{n} clusters. The VIP and VEA calculations analysis shows that the clusters with large size exhibit high metallic character. Consequently, they will liberate more energy when they gain one electron. The chemical hardness shows that the clusters with small size are less reactive and more stable. PDOS analysis reveal that high value of the average total spin magnetic moment for Ti_{n+1} and FeTi_{n} clusters is due to the contribution of the valence orbitals with a large domination of 3d states.

![Fig. 10 Average interatomic distances \( a_0(Ti-Ti) \) and \( a_0(Fe-Ti) \) as a function of cluster size for Ti_{n+1} and FeTi_{n} (\( n = 1–10 \)) clusters](image-url)
Fig. 11  Total (DOS) and projected density of states (PDOS) for Ti₃, Ti₆, FeTi, FeTi₂, and FeTi₄ clusters.
of Ti and Fe atoms. Finally, we hope that these results will serve as a basic resource for further theoretical and experimental research work on new nanoscale materials.

Author contribution All authors contributed to the study conception and design. R. Haichour and S. Mahout performed the simulation, the calculations of different properties, and their analysis. S. Mahout wrote the first draft of the manuscript, and all authors commented on the previous versions of the manuscript. All authors read and approved the final manuscript.

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Data availability The datasets generated during the current study are available from the corresponding author on reasonable request.

Code availability We used the free code SIESTA for all calculations reported in this study.

Conflict of Interest The authors declare no competing interests.

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