

# Optimized interaction parameters for metal-doped endohedral fullerene

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**Abstract** Interaction between various atoms doped inside  $C_{60}$  can be modeled using interaction potentials and, thus, cohesive energy and other physical constants may be calculated. In case of metal-doped fullerene total energy may be written in terms of three different types of interactions, namely carbon–carbon interaction, metal–metal interaction and carbon–metal interaction. Brenner potential, Gupta potential, and Lennard–Jones potentials have been used to model these interactions respectively. Generally, parameters used in these model potentials are not readily available and need to be fine-tuned for different dopants. In this paper, we have deduced/optimized these interaction parameters for Cu, Ag, Al and Ga doped  $C_{60}$  comparing with our Density Functional Theory (DFT) results and hence predicting the stability of various metal-doped fullerenes. Total energy calculations reveal that a maximum of nine copper atoms can be doped inside the fullerene cage and form stable complex without distorting the cage significantly. As we add more number of Cu atoms in the fullerene molecule, cage structure breaks down. In the same way, we have done calculations for Ag, Al and Ga atoms doped inside the fullerene molecule and found that the maximum of eight, nine, nine atoms can form stable complexes.

**Keywords** Fullerene · Metals · DFT · Model potentials

## Introduction

Carbon is an important element known from ancient times and exists in a variety of forms like diamond, graphite, conducting and semiconducting nanotubes and fullerenes. In the recent past closed cage fullerenes have attracted researchers due to their unique structures and properties. The fullerene molecule is having a structure of regular truncated icosahedron. It has 60 carbon atoms located at the vertices of a truncated icosahedron. The icosahedron structure has 90 edges of same length, 60 identical vertices, 20 hexagonal faces and 12 pentagonal faces to form a closed cage (Dresselhaus and Eklund PC 1996). The boundary between a hexagon and a pentagon is a single carbon–carbon bond of bond length 1.41 Å and between two hexagons is a double bond of bond length 1.46 Å. Because of the large size of fullerene molecule as compared to alkali metal dopant atoms or ions, the inner cavity in a  $C_{60}$  molecule can accommodate numerous guest species.

Various concepts have been developed to manipulate, design, characterize and to understand the potential of fullerene as a building block for stable electron donor–acceptor hybrids and conjugates (Nierengarten et al. 2003; Guldi 2003; El-Khouly et al. 2004; Guldi et al. 2004; Segura et al. 2005). Doping is a very famous and effective method for changing the properties of many materials. So Fullerene has been extensively doped (Basiuk et al. 2012; Celasu 2013) to tailor its properties. When fullerene is doped with different atoms, it can change the properties of the system by enhancing their chemical reactivity but the stability of structures is maintained. Exohedral-doped fullerene has shown superconductivity in fullerenes (Hebard et al. 1991). Endohedral metallofullerenes can accommodate additional atoms in them (Akasaka et al. 2010). These fullerenes form interesting complexes that are formed due to electron transfer between

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the fullerene cage and the inner species. Endohedral metallofullerenes are more interesting due to their significant control over the chemical and physical properties, which can be obtained by just changing the nature and composition of doped species (Guldi et al. 2009; Rudolf et al. 2012; Lu et al. 2011). Modeling techniques help in a better way to understand the physical properties of fullerenes and its derivatives. In the literature ab initio calculations have been used to study the structural and electronic properties of small silicon clusters as well as endohedral metallofullerenes (Andreoni 1993; Ibrahim et al. 2006). Ab initio calculations on the stability of  $MC_{60}$  ( $M = Sc, Y$  and  $K$ ) and Si atom-doped endohedral  $C_{60}$  have been reported in the literature (Misra et al. 2012; Suzuki et al. 1994; Ibrahim and El-Haes 2005; Lu et al. 2001). Furthermore, doping of radioactive elements, such as beryllium (Be) (Ohtsuki et al. 1996) and gadolinium (Gd) (Kubozono et al. 1996), has been found to be properly encaged inside a  $C_{60}$  cluster, leading to substantial applications in nuclear waste disposal such as nano-container radio activities. Indeed, the discovery of fullerenes has opened the gate for the production and investigation of much more suitable material building blocks, which could be used as drug deliverers in medical applications and/or possible superconductors in technological applications (Alzahrani 2012). Therefore, fullerene provides an entirely new branch of chemistry, materials science, and physics. Moreover, solid fullerene is treated as a semiconductor material (Saito and Oshiyama 1991).

Large clusters of Cu, Ag, Au, Al and Ga have been extensively studied using tight binding model (Cleri and Rosato 1993). Calculation of cohesive energy and bulk properties of alkali-doped  $C_{60}$  solids with 6-exponential potential is reported (Kumar et al. 2005). Structural and thermodynamic properties of dimer  $C_{60}$  fullerene solid are extensively studied with 6-exponential potential (Kaur et al. 2000). Structural properties of armchair single-wall carbon nanotubes under hydrostatic pressure is reported using Tersoff potential (Imtani and Jindal 2005). Endohedral doped  $C_{60}$  with Si, Ge, Au and Tl has been studied with DFT study and model potentials by our group (Umran and Kumar 2014; Umran et al. 2015). In the present work, we have studied structural properties of  $C_{60}$  fullerene molecule doped with Cu, Ag, Al and Ga atoms using model potentials and compared the results of BE/dopant atom with DFT study done with SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code.

## Model potentials

In case of metal-doped fullerene total energy may be written in terms of three different types of interactions, namely carbon–carbon interaction, metal–metal interaction

and carbon–metal interaction. Brenner potential, Gupta potential, and Lennard–Jones potentials have been used to model these interactions, respectively. Generally parameters used in these model potentials are not readily available and need to be fine-tuned for different dopants. Brenner potential (Brenner 1990) has been used to study properties of several carbon based systems like graphite, diamond, fullerenes and carbon nanotubes (Gupta et al. 2005; Robertson et al. 1994). The interaction between carbon and metal is calculated by Lennard–Jones potential (Guan et al. 1996), the interaction between metal–metal is calculated by Gupta potential (Gupta 1981). These potentials have been used for calculating the ground state energies of endohedral fullerenes (Umran et al. 2015). Total energy of the metal-doped endohedral fullerene may be written as

$$E = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j \\ C-C}} V_{ij}^B + \frac{1}{2} \sum_{\substack{i,j \\ C-M}} V_{ij}^{L-J} + V_{M-M}^G, \quad (1)$$

where  $V_{ij}^B$  (Brenner potential) corresponds to the energy between carbon–carbon atoms.  $V_{ij}^{L-J}$  (Lennard–Jones potential) is the energy between carbon–metal atoms and  $V_{M-M}^G$  (Gupta potential) is the energy between metal–metal atoms. Total energy of the pristine fullerene may be expressed as

$$E_{C60} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j \\ C-C}} V_{ij}^B \quad (2)$$

Binding energy/dopant becomes  $BE = \frac{E - E_{C60}}{No. of dopants}$ . The potentials used are briefly described in the following section.

## Brenner potential

Brenner potential is a class of empirical potentials used to model covalently bound systems. Thus, Brenner potential is able to describe the physical properties for compound interactions correctly. The potential energy between any two carbon atoms on  $C_{60}$ , say  $i$  and  $j$ , separated by a distance  $r_{ij}$  is given as:

$$V_{ij}^B = V_R(r_{ij}) - B_{ij} V_A(r_{ij}), \quad (3)$$

where

$$V_R(r_{ij}) = f(r_{ij}) \left[ \frac{D_{ij}^{(e)}}{S_{ij} - 1} \right] \exp \left[ -\beta_{ij} \sqrt{2S_{ij}} \left( r - R_{ij}^{(e)} \right) \right] \quad (4)$$

$$V_A(r_{ij}) = f(r_{ij}) \left[ \frac{D_{ij}^{(e)} S_{ij}}{S_{ij} - 1} \right] \exp \left( -\beta_{ij} \sqrt{\frac{2}{S_{ij}}} (r - R_{ij}^{(e)}) \right) \quad (5)$$

$$f(r_{ij}) = \begin{cases} 1, & \text{if } r_{ij} < R_{ij}^{(1)} \\ \frac{1}{2} \left[ 1 + \cos \left( \frac{\pi (r_{ij} - R_{ij}^{(1)})}{R_{ij}^{(2)} - R_{ij}^{(1)}} \right) \right], & \text{if } R_{ij}^{(1)} < r_{ij} < R_{ij}^{(2)} \\ 0, & \text{if } r_{ij} > R_{ij}^{(2)} \end{cases} \quad (6)$$

Here,  $V_R$  and  $V_A$  are the repulsive and attractive potential energy terms, respectively.  $R_{ij}^{(e)}$  is the equilibrium distance between atoms  $i$  and  $j$ .  $S_{ij}, D_{ij}^{(e)}, \beta_{ij}$  are the constants that reflects the types of atoms  $i$  and  $j$ . The screening function  $f(r_{ij})$  restricts the interaction to nearest neighbors as defined by the values of  $R_{ij}^{(1)}$  and  $R_{ij}^{(2)}$ . In addition, the Brenner potential takes bonding topology into account with empirical bond order function  $B_{ij}$ . Table 1 shows the parameter set for the Brenner empirical potential (Brenner 1990).

### Lennard–Jones potential

Lennard–Jones potential is employed to model the van der Waals effect in molecular collision simulations. The form of the Lennard–Jones potential is very similar to.

$$V_{ij}^{L-J} = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] \quad (7)$$

Here  $\sigma$  corresponds to the distance between two atoms at equilibrium and  $\varepsilon$  represents the strength of interaction. The optimized parameters ( $\varepsilon, \sigma$ ) for Cu–C, Ag–C, Al–C and Ga–C used in present calculations are listed in Table 2.

### Gupta potential

The many-body Gupta potential is used to study the structure and properties of metal–metal clusters. Gupta potential is derived from Gupta's expression (Gupta 1981) for the cohesive energy of bulk material. It includes a repulsive pair  $V_{ij}^r$  and many-body attractive terms  $V_{ij}^m$ .

$$V^G = \sum_{i=1}^N \left[ \sum_{\substack{j=1 \\ j \neq i}}^N V_{ij}^r(r_{ij}) - \sqrt{\sum_{\substack{j=1 \\ j \neq i}}^N V_{ij}^m} \right], \quad (8)$$

$$V_{ij}^r = A \exp \left( -p_{ij} \left[ \frac{r_{ij}}{r_0} - 1 \right] \right), \quad (9)$$

$$V_{ij}^m = \zeta^2 \exp \left( -2q_{ij} \left[ \frac{r_{ij}}{r_0} - 1 \right] \right), \quad (10)$$

where  $r_{ij}$  is the distance between two atoms  $A$ ,  $r_0, \zeta, p, q$  are the parameters fitted to experimental values of the cohesive energy, lattice parameters and independent of elastic constants for the reference crystal at 0 K. The Gupta potential parameters used in present calculations are listed in the Table 3.

## Results and discussion

In this part, we show the optimized structures of  $M_n@C_{60}$  ( $M = \text{Cu, Ag, Al and Ga}$ ) molecules. Initial input coordinates of pure  $C_{60}$  fullerene molecule and doped fullerenes have been taken from DFT calculations (Dhiman et al. 2015). Then the calculations were done using model potentials as discussed in “Model potentials” section. The parameters for model potential calculations have been taken from the literature and the calculations have been done for structural analysis and BE/dopant atom. We observed that the result for BE/dopant atom differ much from the result obtained from DFT study calculations. Then we tune few parameters like  $R_{ij}^{(2)}$  and  $r_0$  as shown in Table 2 and Table 3. The results obtained with new parameters are in excellent agreement with DFT calculations. The calculated values of single and double bonds in fullerene molecule are between 1.41 and 1.46 Å, respectively. These values are in good agreement with the experimental values between 1.40 and 1.46 Å (Hedberg et al. 1991). First, we focus on the study of structural properties of copper and silver doped fullerenes and then

**Table 1** The parameters of Brenner Potential (Brenner 1990)

$D_{ij}^{(e)}$ (eV)	$S_{ij}$	$\beta_{ij} \text{ \AA}^{(-1)}$	$\delta_{ij}$	$R_{ij}^e$ (Å)	$R_{ij}^{(1)}$ (Å)	$R_{ij}^{(2)}$ (Å)	$a_0$	$c_0$	$d_0$
6.325	1.29	1.5	0.80469	1.315	1.7	2.0	0.011304	19	2.5

**Table 2** Lennard–Jones potential parameters

Parameter	Cu–C	Ag–C	Al–C	Ga–C
$\varepsilon$ (eV)	0.3596	0.3250	0.3290	0.3540
$\sigma$ (Å)	1.503	1.444	1.570	1.545

**Table 3** Gupta potential parameters

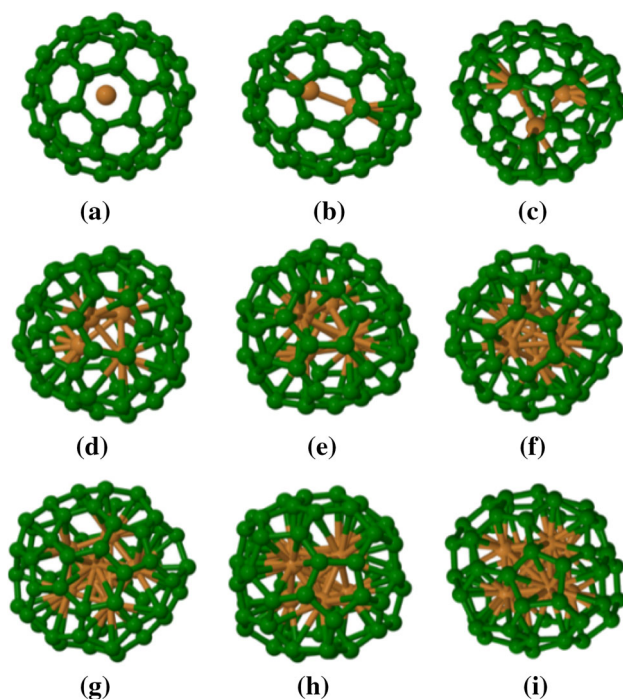
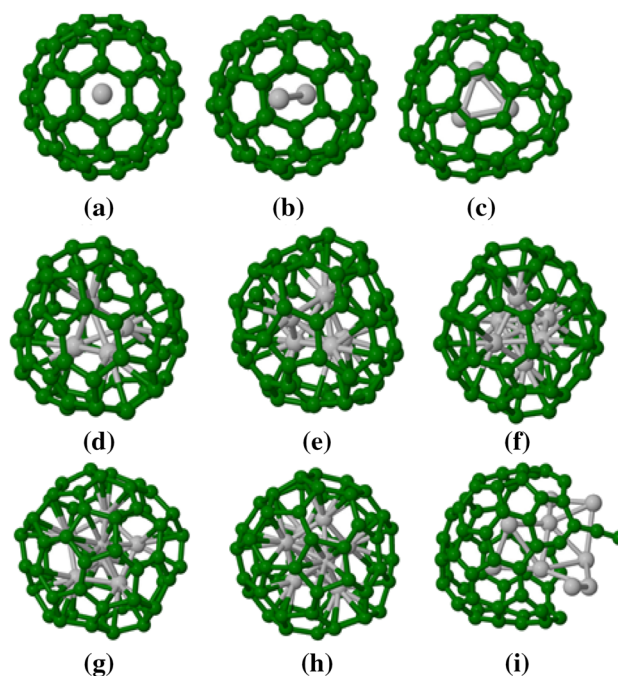
Parameter	Cu–Cu	Ag–Ag	Al–Al	Ga–Ga
A (eV)	0.0855	0.1206	0.1221	0.1210
$\zeta$ (eV)	1.2240	1.1895	1.316	1.318
p	10.960	10.850	8.612	8.713
q	2.2780	3.180	2.516	2.416
$r_o$ (Å)	2.998	2.790	3.201	2.125

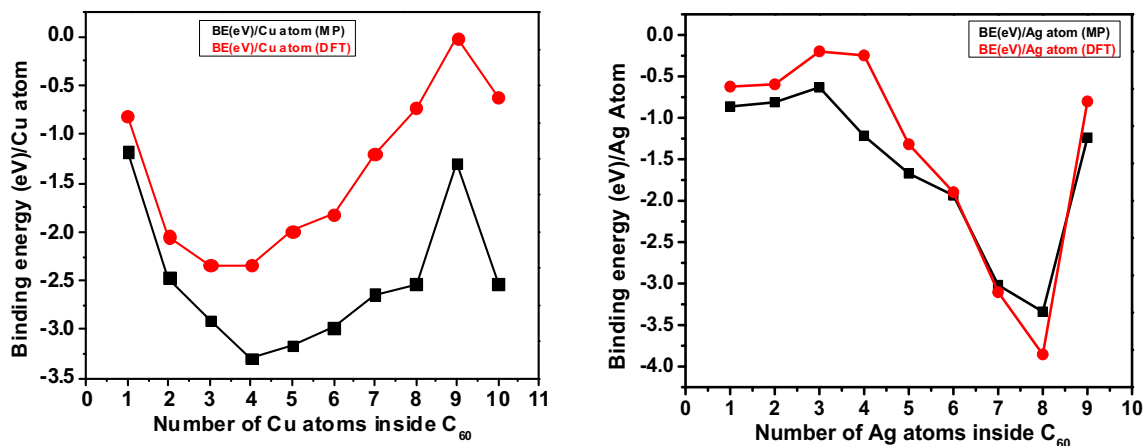
aluminum- and gallium-doped fullerenes have been discussed.

### Cu and Ag atoms doped inside $C_{60}$ (Group II elements)

The optimized fullerene structure is used to dope copper and silver atoms. First of all, initial coordinates are

assigned to copper and carbon atoms of  $C_{60}$  molecule and the system was allowed to relax without additional constraints. The ground state structures of copper-doped fullerenes are shown in Fig. 1. In  $Cu_1@C_{60}$  complex single copper atom stabilizes in the center of  $C_{60}$  (Fig. 1a). In  $Cu_2@C_{60}$  structure two Cu atoms exist in a dimer form having Cu–Cu bond distance is 2.22 Å inside the fullerene cage. The dimer lies in the center of two hexagons of the fullerene ring (Fig. 1b). Bond length of dimer as calculated by DFT study is 2.16 Å. There is only a difference of 0.06 Å between the two calculations. The carbon–copper bond distance is 2.59 Å. In case of  $Cu_3@C_{60}$ ,  $Cu_3$  exist in triangular structure (Fig. 1c) with copper–copper bond distance 2.23 Å and carbon–copper bond distance varies from 2.65 to 2.69 Å. In  $Cu_4@C_{60}$ ,  $Cu_4$  shows a tetrahedron structure (Fig. 1d) with copper–copper and carbon–copper bond lengths of 2.21 and 2.63 Å respectively. In  $Cu_5@C_{60}$ , cluster of five copper atoms shows a stable triangular bipyramidal structure lies in the center of  $C_{60}$  with copper–copper and carbon–copper bond lengths 2.3, 2.1 and 2.47–2.58 Å respectively as presented in (Fig. 1e). Cluster of  $Cu_6$  in  $Cu_6@C_{60}$  exist in a square bipyramid (Fig. 1f) form lies symmetrically in the center of two hexagons with copper–copper and carbon–copper bond lengths 2.13, 2.15 and 2.43–2.64 Å.  $Cu_7@C_{60}$  form a stable structure with  $Cu_7$  has a perfect pentagonal

**Fig. 1** Ground state structures of  $Cu_n@C_{60}$  ( $n = 1–9$ )**Fig. 2** Ground state structures of  $Ag_n@C_{60}$  ( $n = 1–9$ )

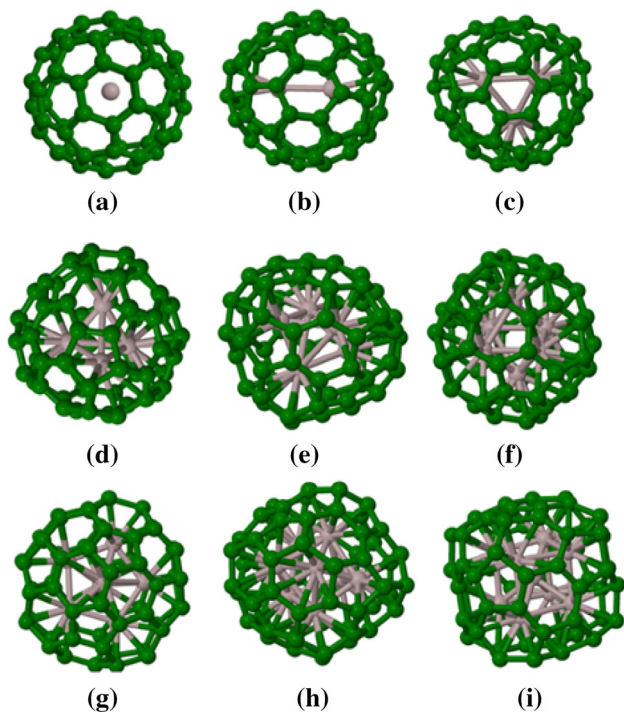


**Fig. 3** Variation of BE/Cu or Ag atom with number of atoms

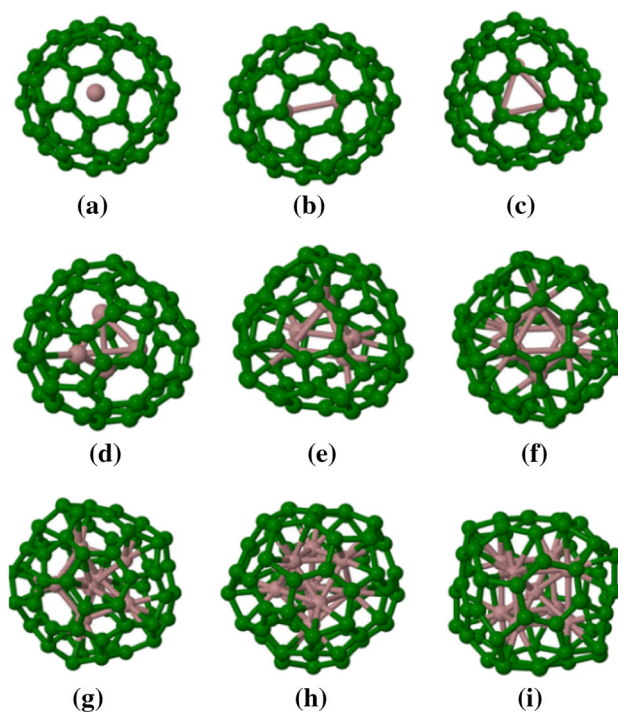
bipyramidal structure having copper–copper and carbon–copper bond lengths 2.04, 2.18, 2.40–2.67 Å respectively (Fig. 1g). In Cu<sub>8</sub>@C<sub>60</sub> complex (Fig. 1h), Cu<sub>8</sub> forms a distorted cube of copper–copper bond length varies from 2.03–2.06 Å and all copper atoms form bonds with carbon atoms of the cage having carbon–copper bond length varies from 2.37–2.63 Å and in Cu<sub>9</sub>@C<sub>60</sub> (Fig. 1i), Cu<sub>9</sub> shows a body centered cube with copper–copper bond length 2.17 Å, the body centered copper atom is at a distance of 1.93 Å from other two copper atoms situated at the diagonal and carbon–copper bond length varies

from 2.37–2.56 Å, respectively. Doping of 10th copper atom in the fullerene molecule exerts a strain in carbon–carbon bond and the cage breaks. As the size of copper clusters inside the fullerene increases, distortion of cage increases as it cannot withstand the pressure exerted by cluster atoms.

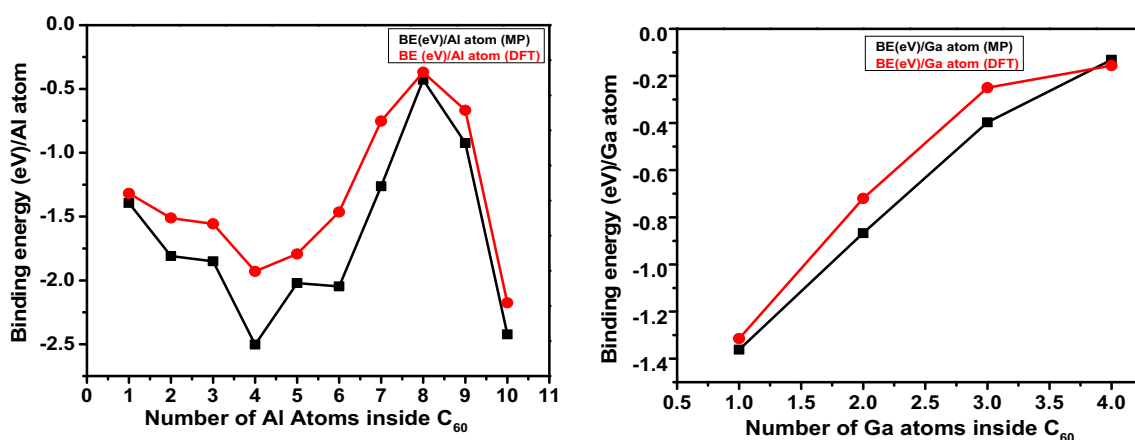
In the same way, we have done doping of Ag atoms in the C<sub>60</sub> cage and the ground state structures of Ag<sub>n</sub>@C<sub>60</sub> ( $n = 1–9$ ) are presented in Fig. 2. On doping of single Ag atom in the fullerene molecule produce Ag<sub>1</sub>@C<sub>60</sub> complex. Ag atom is placed at different positions inside the cage and



**Fig. 4** Ground state structures of Al<sub>n</sub>@C<sub>60</sub> ( $n = 1–9$ )



**Fig. 5** Ground state structures of Ga<sub>n</sub>@C<sub>60</sub> ( $n = 1–9$ )



**Fig. 6** Variation of BE/Al or Ga atom with number of atoms

found that is stable only in the center of the C<sub>60</sub> molecule. Encapsulation of two Ag atoms inside the fullerene cage leads to the formation of Ag<sub>2</sub>@C<sub>60</sub> complex. In this case Ag<sub>2</sub> dimer is stable like Cu<sub>2</sub> dimer and lies symmetrically in the center of two hexagons of the cage. Ag<sub>2</sub> molecule does not make any bond with carbon atom of the fullerene.

The calculated Ag–Ag interatomic distance is 2.38 Å, which is 0.17 Å less than bare optimized Ag<sub>2</sub> dimer. In Ag<sub>3</sub>@C<sub>60</sub>, Ag<sub>3</sub> has a triangular structure similar to Cu<sub>3</sub>@C<sub>60</sub>. The bond length of Ag–Ag dimer is 2.41 Å and this structure does not form any bond with carbon atom of the cage. In the case of Ag<sub>4</sub>@C<sub>60</sub>, Ag<sub>4</sub> has a tetrahedron structure with silver–silver bond length 2.45 Å and all the four Ag atoms form bond with carbon atoms of the cage with carbon–silver bond length 2.70 Å. Ag<sub>5</sub> in Ag<sub>5</sub>@C<sub>60</sub> exist as a trigonal bipyramid structure with bond lengths 2.62 and 2.41 Å. All the five silver atoms form bonds with carbon atoms of the cage with bond length 2.65 Å. In Ag<sub>6</sub>@C<sub>60</sub> complex, Ag<sub>6</sub> cluster has a square bipyramid structure with silver–silver and carbon–silver bond lengths 2.46, 2.45 and 2.67 Å respectively. Inside Ag<sub>7</sub>@C<sub>60</sub> complex, Ag<sub>7</sub> cluster form a pentagon bipyramid structure, silver–silver and carbon–silver bond lengths are 2.33, 2.59–2.68 Å respectively. In Ag<sub>8</sub>@C<sub>60</sub> complex, Ag<sub>8</sub> form a distorted cube with Ag–Ag bond length varies from 2.33–2.41 Å. All eight Ag atoms form bonds with carbon atoms of the fullerene cage and carbon–silver bond length varies from 2.59–2.71 Å.

On doping of cluster of nine silver atoms, the C<sub>60</sub> cage breaks as shown in Fig. 2a. The variation of BE/dopant atom of Cu<sub>n</sub>@C<sub>60</sub> and Ag<sub>n</sub>@C<sub>60</sub> with number of dopant atoms as calculated with model potentials and with DFT study is plotted in Fig. 3. The results indicate that the reported parameters have reproduced DFT results (Dhiman et al. 2015) qualitatively as well as quantitatively. Therefore, the model of interactions and new parameters describes endohedral systems with great accuracy.

### Doping of Al and Ga atoms inside C<sub>60</sub> (group III elements)

The relaxed structures of Al<sub>n</sub>@C<sub>60</sub> ( $n = 1–9$ ) and Ga<sub>n</sub>@C<sub>60</sub> ( $n = 1–9$ ) are presented in Figs. 4 and 5. The calculated Al–Al bond distance in relaxed structure is 2.59 Å. This is almost 0.1 Å less than the value reported (Wang et al. 2000) and agreed well with the experimental value 2.56 Å (Rosen 1970). The Calculated Ga–Ga interatomic distance is found to be 2.62 Å, which is 0.06 Å less than the value reported (Balasubramanian 1990). In both cases it is found that the fullerene complexes are stable up to  $n = 1–9$  with a small distortion of the cage due to large size of dopant clusters. But on addition of tenth aluminum or gallium atom inside the C<sub>60</sub> cage, it breaks.

This is due to the fact that the empty space inside C<sub>60</sub> is not sufficient to accommodate large clusters. It is also inferred that the stability of the fullerene cage generally depend upon the number of dopant atoms (Al, Ga) atoms inside the cage. BE/dopant atom (Al/Ga) of Al<sub>n</sub>@C<sub>60</sub> and Ga<sub>n</sub>@C<sub>60</sub> ( $n = 1–10$ ) with number of dopant atoms as calculated with model potentials and DFT study is presented in Fig. 6. We found that the BE/Al atom follow the same trend as we have found in DFT calculations.

In case of Ga-doped fullerene, BE/Ga atom decreases up to four Ga atoms and then it becomes positive. This implies that complexes are in metastable state and still preserve the symmetry and cage breaks only after insertion of tenth gallium atom. So the results obtained with potential calculations are in good agreement with the DFT study and again establishes the authenticity of model potentials and new set of interaction parameters. From the structure analysis it is found that the stability of fullerene shell strongly depends upon the number of dopant atoms in the cage.

## Conclusions

In the present paper, we have investigated the structures and BE/dopant of Cu, Ag, Al and Ga doped endohedral fullerenes with the help of model potentials. Brenner potential, Lennard–Jones potential and Gupta potential are used to study carbon–carbon, carbon–metal and metal–metal interactions. Total energy calculations have been done to find out the ground state energy structures and BE/dopant atom. In  $Cu_n@C_{60}$  molecule, maximum nine copper atoms can be doped inside the fullerene cage and form stable complexes without distorting the cage significantly. The addition of tenth copper atom inside the cage increases the size of the copper cluster and produces a large pressure on the wall of the cage. As a result, the strength of carbon–carbon bonds become weak and this leads to the breaking of fullerene cage. The space inside the fullerene cage is not sufficient to accommodate large size clusters beyond nine atoms. Similarly maximum eight silver atoms, nine aluminum atoms and nine gallium atoms can be doped inside the fullerene cage those can make stable complexes. The calculated values of BE/dopant atom with model potentials are in excellent agreement with the values calculated with DFT study. This validates our results of model potentials and new set of interaction parameters.

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## References

- Akasaka T, Wudl F, Nagase S (2010) Chemistry of nanocarbons. Wiley, Chichester, UK
- Alzahrani AZ (2012) International Scholarly Research Network ISRN. Condens Mat Phys. doi:10.5402/2012/208234

- Andreoni W (1993) Nanostruct Mater 3:293–300
- Balasubramanian K (1990) J Phys Chem 94:7764
- Basiuk VA, Cruz-Gregorio A (2012) J Comp Theor Nanosci 9:922
- Brenner DW (1990) Phys Rev B 42:9458
- Celasu S (2013) Rev Theor Sci 1:319
- Cleri F, Rosato V (1993) Phys Rev B 48:22
- Dhiman S, Kumar R, Dharmvir K (2015) J Molecul Struct 1100:328–337
- Dresselhaus MS, Dresselhaus G, Eklund PC (1996) Science of Fullerenes and Carbon Nanotubes. Academic Press
- El-Khouly ME, D'Souza F, Ito O (2004) J Photochem Photobiol C 5:79–104
- Guan P, RMckenzie D, Pailthorpe BA (1996) J Phys Condens Matter 8:8753–8762
- Guldi DM (2003) Pure Appl Chem 75:1069–1107
- Guldi DM, Prato M (2004) Chem Commun 22:2517–2525
- Guldi DM, Martín, Feng L, Akasaka T, Nagase S (2009) Endohedrals 455–490
- Gupta RP (1981) Phys Rev B 23:6265
- Gupta S, Dharmvir K, Jindal VK (2005) Phys Rev B 72:165428
- Hebard AF, Rosseinsky MJ, Haddon RC, Murphy DW, Glarm SH, Palstra TTM, Ramirez AP, Kortan AR (1991) Nature 350:600
- Hedberg K, Hedberg L, Bethune DS, Brown CA, Dorn HC, Johnson RD, de Vries M (1991) Science 254:410
- Ibrahim M, El-Haes H (2005) Chin J Phys 43:915
- Ibrahim M, El-Haes H, Jalbout AF (2006) Chin J Phys 44:432–439
- Imtani AN, Jindal VK (2007) Phys Rev B 76:195447
- Kaur N, Bajwa N, Dharmvir K, Jindal VK (2000) Inter J Mod Phys B 14:2597–2607
- Kubozono Y, Maeda H, Takabayashi Y (1996) Isolation and characterization of  $C_{60}$ . J Amer Chem Soc 118:6998–6999
- Kumar R, Dharmvir K, Jindal VK (2005) Phys B 365:121
- Lu J, Zhou Y, Zhang S, Zhang X, Zhao X (2001) Chem Phys Lett 343:39–43
- Lu X, Akasaka T, Nagase S (2011) Chem Commun 47:5942–5957
- Misra N, Dwivedi A, Pandey A (2012) Chin J Phys 50:64–72
- Nierengarten JF (2003) Top Curr Chem 228:87–110
- Ohtsuki T, Masumoto K, Ohno K (1996) Phys Rev Lett 77:3522–3524
- Robertson DH, Brenner DW, White CT (1994) J Phys Chem 99:15721
- Rosen B (1970) Spectroscopic data relative to diatomic molecules. Pergamon, Oxford
- Rudolf M, Wolfrum S, Guldi DM, Feng L, Tsuchiya T, Akasaka T, Echegoyen L (2012) J Eur Chem 18:5136–5148
- Saito S, Oshiyama A (1991) Phys Rev Lett 66:2637–2640
- Segura JL, Martín ND, Guldi M (2005) Chem Soc Rev 34:31–47
- Suzuki S, Torisu H, Kubota H, Wakabayashi T, Shiromaruand H, Achiba Y (1994) Int J Mass Spectrom 138:297–300
- Umran NM, Kumar R (2014) Physica B 437:47–52
- Umran NM, Kaur N, Seema K, Kumar R (2015) Mater Res Express 2:055603
- Wang M, Huang X, Zuliang Du, Yuncai Li (2000) Chem Phys Lett 480:258–264