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# Assessing a double silicon decorated fullerene for the delivery of interacting flurbiprofen and salicylic acid drugs: A DFT approach

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**Abstract**

Since the number of drugs increases constantly, drug interactions appear as a critical issue to handle. The effective use of multiple drugs appears as another important subject to discuss and the use of targeted and selective delivery of drugs is becoming more important. Impurity doped C<sub>60</sub> fullerenes with various dopant atoms such as silicon or boron appear as promising drug delivery vehicles. Therefore, in the framework of this study, we investigated the interaction between salicylic acid and flurbiprofen and their controlled delivery by using double silicon decorated C<sub>60</sub> fullerene using density functional theory. Stability and reactivity considerations were also examined by investigating some important structural parameters, interaction energies and frontier molecular orbitals. The interactions were also monitored by examining important diagnostic vibrational bands. The strength of the interactions between atoms at the interaction sites was also identified by using the quantum theory of atoms in molecules. © 2023 Indian Chemical Society

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DFT; Flurbiprofen; Fullerene; QTAIM; Salicylic acid

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- 1 Seymour, R.M., Routledge, P.A.  
**Important drug-drug interactions in the elderly**

(1998) *Drugs and Aging*, 12 (6), pp. 485-494. Cited 148 times.  
doi: 10.2165/00002512-199812060-00006

[View at Publisher](#)

- 2 Prichard, M.N., Shipman Jr., C.  
**A three-dimensional model to analyze drug-drug interactions**

(1990) *Antiviral Research*, 14 (4-5), pp. 181-205. Cited 500 times.  
doi: 10.1016/0166-3542(90)90001-N

[View at Publisher](#)

- 3 Zhang, Y., Qiu, Y., Cui, Y., Liu, S., Zhang, W.  
**Predicting drug-drug interactions using multi-modal deep auto-encoders based network embedding and positive-unlabeled learning**

(2020) *Methods*, 179, pp. 37-46. Cited 36 times.  
<http://www.elsevier.com.mapua.idm.oclc.org/inca/publications/store/6/2/2/9/1/4/index.htm>  
doi: 10.1016/j.meth.2020.05.007

[View at Publisher](#)

- 4 Brown, J.D., Winterstein, A.G.  
**Potential adverse drug events and drug–drug interactions with medical and consumer cannabidiol (CBD) use**

(2019) *Journal of Clinical Medicine*, 8 (7), art. no. 989. Cited 138 times.  
<https://www.mdpi.com/2077-0383/8/7/989/pdf>  
doi: 10.3390/jcm8070989

[View at Publisher](#)

- 5 Younis, I.R., Lakota, E.A., Volpe, D.A., Patel, V., Xu, Y., Sahajwalla, C.G.  
**Drug-Drug Interaction Studies of Methadone and Antiviral Drugs: Lessons Learned**

(2019) *Journal of Clinical Pharmacology*, 59 (8), pp. 1035-1043. Cited 11 times.  
[http://onlinelibrary.wiley.com.mapua.idm.oclc.org/journal/10.1002/\(ISSN\)1552-4604](http://onlinelibrary.wiley.com.mapua.idm.oclc.org/journal/10.1002/(ISSN)1552-4604)  
doi: 10.1002/jcpb.1405

[View at Publisher](#)

- 6 Zhang, H., Ma, L., Jiang, S., Lin, H., Zhang, X., Ge, L., Xu, Z.  
**Enhancement of biocontrol efficacy of Rhodotorula glutinis by salicylic acid against gray mold spoilage of strawberries**

(2010) *International Journal of Food Microbiology*, 141 (1-2), pp. 122-125. Cited 29 times.  
doi: 10.1016/j.ijfoodmicro.2010.04.022

[View at Publisher](#)

- 7 Kovács, A., Berkó, S., Csányi, E., Csóka, I.  
**Development of nanostructured lipid carriers containing salicylic acid for dermal use based on the Quality by Design method**

(2017) *European Journal of Pharmaceutical Sciences*, 99, pp. 246-257. Cited 44 times.  
[www.elsevier.com/locate/ejps](http://www.elsevier.com/locate/ejps)  
doi: 10.1016/j.ejps.2016.12.020

[View at Publisher](#)

- 8 Valentovic, M.  
Flurbiprofen, xPharm: the Comprehensive Pharmacology Reference  
(2007), pp. 1-6. Cited 136 times.

Scival topics

Chemicals and CAS  
Registry Numbers

- 9 Salata, O.V.  
**Applications of nanoparticles in biology and medicine**  
(2004) *Journal of Nanobiotechnology*, 2, art. no. 3. Cited 1812 times.  
<http://www.jnanobiotechnology.com/content/2/1/3>  
doi: 10.1186/1477-3155-2-3

[View at Publisher](#)

- 10 Pantarotto, D., Partidos, C.D., Hoebeke, J., Brown, F., Kramer, E., Briand, J.-P., Muller, S., (...), Bianco, A.

**Immunization with peptide-functionalized carbon nanotubes  
enhances virus-specific neutralizing antibody responses**

(2003) *Chemistry and Biology*, 10 (10), pp. 961-966. Cited 499 times.  
<http://www.cell.com>  
doi: 10.1016/j.chembiol.2003.09.011

[View at Publisher](#)

- 11 Hatami, A., Heydarinasab, A., Akbarzadehkhiyavi, A., Shariati, F.P.  
An introduction to nanotechnology and drug delivery  
(2021) *Chem. Methodol.*, 5, pp. 153-165. Cited 32 times.

Scival topics

Chemicals and CAS  
Registry Numbers

- 12 Harismah, K., Shahrtash, S.A., Arabi, A.R., Khadivi, R., Mirzaei, M., Akhavan-Sigari, R.  
**Favipiravir attachment to a conical nanocarbon: DFT assessments  
of the drug delivery approach** (Open Access)

(2022) *Computational and Theoretical Chemistry*, 1216, art. no. 113866. Cited 10 times.  
<http://www.sciencedirect.com.mapua.idm.oclc.org/science/journal/2210271X/970>  
doi: 10.1016/j.comptc.2022.113866

[View at Publisher](#)

- 13 Saadh, M.J., Amin, A.H., Farhadiyan, S., Sadeghi, M.S., Shahrtash, S.A., Maaliw, R.R., Saimmai Hanaf, A., (...), Akhavan-Sigari, R.  
**Sensing functions of an iron-doped boron nitride nanocone  
towards acetaminophen and its thio/thiol analogs: A DFT outlook**

(2023) *Diamond and Related Materials*, 133, art. no. 109749. Cited 3 times.  
<https://www.journals.elsevier.com/diamond-and-related-materials>  
doi: 10.1016/j.diamond.2023.109749

[View at Publisher](#)

- 14 Darougari, H., Rezaei-Sameti, M.  
The drug delivery appraisal of Cu and Ni decorated  $B_{12}N_{12}$  nanocage for an 8-hydroxyquinoline drug: a DFT and TD-DFT computational study  
(2022) *Asian J. Nanosci. Mater.*, 5, pp. 196-210. Cited 16 times.

Scival topics

Chemicals and CAS  
Registry Numbers

- 15 Aghazadeh, H., Taheri, P., Hassani, S., Sangchooli, T., Ouni, M., Asghari, N.  
**Vancomycin prolonged release via PLGA system loaded with drug-containing chitosan nanoparticles as a novel in situ forming drug delivery system**

(2023) *Eurasian Chemical Communications*, 5 (5), pp. 392-403. Cited 3 times.  
[http://www.echemcom.com/article\\_164885\\_d4fc2ad938a12049611cccc12faa555b.pdf](http://www.echemcom.com/article_164885_d4fc2ad938a12049611cccc12faa555b.pdf)

Scival topics

- 16 Ghasemi Gol, A., Akbari, J., Khalaj, M., Mousavi-Safavi, S.M., Esfahani, S., Farahani, N.

**DFT investigation of a Zn-doped carbon nanocone for the drug delivery of methylated aspirins**

(2023) *Computational and Theoretical Chemistry*, 1220, art. no. 113976. Cited 2 times.

<http://www.sciencedirect.com.mapua.idm.oclc.org/science/journal/2210271X/970>  
doi: 10.1016/j.comptc.2022.113976

[View at Publisher](#)

SciVal topics

- 17 Bakry, R., Vallant, R.M., Najam-ul-Haq, M., Rainer, M., Szabo, Z., Huck, C.W., Bonn, G.K.

**Medicinal applications of fullerenes**

(2007) *International Journal of Nanomedicine*, 2 (4), pp. 639-649. Cited 664 times.

- 18 Clemmer, D.E., Hunter, J.M., Shelimov, K.B., Jarrold, M.F.

**Physical and chemical evidence for metallofullerenes with metal atoms as part of the cage (Open Access)**

(1994) *Nature*, 372 (6503), pp. 248-250. Cited 124 times.

doi: 10.1038/372248a0

[View at Publisher](#)

SciVal topics

- 19 Antonietti, M., Müllen, K.

**Chemical synthesis and applications of graphene and carbon materials**

(2016) *Chemical synthesis and applications of graphene and carbon materials*, pp. 1-256. Cited 15 times.

<http://onlinelibrary.wiley.com.mapua.idm.oclc.org/book/10.1002/9783527648160>  
ISBN: 978-352764816-0; 978-352733208-3

doi: 10.1002/9783527648160

[View at Publisher](#)

SciVal topics

- 20 Billas, I.M.L., Branz, W., Malinowski, N., Tast, F., Heinebrodt, M., Martin, T.P., Massobrio, C., (...), Parrinello, M.

**Experimental and computational studies of heterofullerenes**

(1999) *Nanostructured Materials*, 12 (5), pp. 1071-1076. Cited 51 times.

doi: 10.1016/S0965-9773(99)00301-3

[View at Publisher](#)

- 21 Tomasi, J., Mennucci, B., Cammi, R.

**Quantum mechanical continuum solvation models**

(2005) *Chemical Reviews*, 105 (8), pp. 2999-3093. Cited 12950 times.

<http://pubs.acs.org.mapua.idm.oclc.org/journal/chreay>

doi: 10.1021/cr9904009

[View at Publisher](#)

SciVal topics

- 22 Gutowski, M., Chałasiński, G.

**Critical evaluation of some computational approaches to the problem of basis set superposition error**

(1993) *The Journal of Chemical Physics*, 98 (7), pp. 5540-5554. Cited 151 times.

doi: 10.1063/1.464901

[View at Publisher](#)

- 23 Chojecki, M., Yourdkhani, S., Rutkowska-Zbik, D., Korona, T.  
Stability of endo- and exohedral complexes of all-boron fullerene B<sub>40</sub>

SciVal topics

Chemicals and CAS  
Registry Numbers

(2018) *Computational and Theoretical Chemistry*, 1133, pp. 7-17. Cited 10 times.  
<http://www.sciencedirect.com.mapua.idm.oclc.org/science/journal/2210271X/970>  
doi: 10.1016/j.comptc.2018.04.007

[View at Publisher](#)

- 24 Bader, R.F.W.  
Atoms in Molecules: A Quantum Theory  
(1990). Cited 18869 times.  
Clarendon New York

SciVal topics

Chemicals and CAS  
Registry Numbers

- 25 Rozas, I., Alkorta, I., Elguero, J.  
Behavior of ylides containing N, O, and C atoms as hydrogen bond acceptors

(2000) *Journal of the American Chemical Society*, 122 (45), pp. 11154-11161. Cited 1240 times.  
doi: 10.1021/ja0017864

[View at Publisher](#)

- 26 Lu, T., Chen, F.  
Multiwfn: A multifunctional wavefunction analyzer

(2012) *Journal of Computational Chemistry*, 33 (5), pp. 580-592. Cited 17022 times.  
doi: 10.1002/jcc.22885

[View at Publisher](#)

- 27 Frisch, M.J., Trucks, G.W., Schlegel, H.B.  
Gaussian 09, Revision A.1  
(2009). Cited 30727 times.  
Gaussian Inc. Wallingford, CT

SciVal topics

Chemicals and CAS  
Registry Numbers

- 28 Dennington, R.D., Keith, T.A., Millam, J.M.  
GaussView 5.0.8  
(2008). Cited 2973 times.  
Gaussian Inc.

- 29 Fukui, K.  
Role of frontier orbitals in chemical reactions

(1982) *Science*, 218 (4574), pp. 747-754. Cited 1894 times.  
doi: 10.1126/science.218.4574.747

[View at Publisher](#)

- 30 Ayala, P.Y., Scuseria, G.E.  
Linear scaling second-order Moller-Plesset theory in the atomic orbital basis for large molecular systems

(1999) *Journal of Chemical Physics*, 110 (8), pp. 3660-3671. Cited 361 times.  
<http://scitation.aip.org.mapua.idm.oclc.org/content/aip/journal/jcp>  
doi: 10.1063/1.478256

[View at Publisher](#)

- 31 Sylaja, B., Gunasekaran, S., Srinivasan, S.

SciVal topics

Chemicals and CAS

Registry Numbers

Vibrational, NLO, NBO, NMR, frontier molecular orbital and molecular docking studies of diazepam ([Open Access](#))

(2018) *Materials Research Innovations*, 22 (6), pp. 361-373. Cited 7 times.  
<http://www.tandfonline.com/loi/ymri20#.VwHdSE1fQs>  
doi: 10.1080/14328917.2017.1324356

[View at Publisher](#)

32 Sathy, K., Dhamodharan, P., Dhandapani, M.

Spectral, optical, thermal, Hirshfeld, antimicrobial studies and computational calculations of a new organic crystal, 1H-benzo[d]imidazol-3-ium-3,5-dinitrobenzoate ([Open Access](#))

SciVal topics

Chemicals and CAS

Registry Numbers

(2017) *Journal of Molecular Structure*, 1137, pp. 663-673. Cited 14 times.  
[www.elsevier.com/inca/publications/store/5/0/0/8/5/0/index.htm](http://www.elsevier.com/inca/publications/store/5/0/0/8/5/0/index.htm)  
doi: 10.1016/j.molstruc.2017.02.070

[View at Publisher](#)

33 Sundaram, S., Vijayakumar, V.N., Balasubramanian, V.

Electronic and structure conformational analysis (HOMO-LUMO, MEP, NBO, ELF, LOL, AIM) of hydrogen bond binary liquid crystal mixture: DFT/TD-DFT approach

(2022) *Computational and Theoretical Chemistry*, 1217, art. no. 113920. Cited 2 times.

<http://www.sciencedirect.com.mapua.idm.oclc.org/science/journal/2210271X/970>  
doi: 10.1016/j.comptc.2022.113920

[View at Publisher](#)

34 Mohamed Ahmed, M.S., Mekky, A.E.M., Sanad, S.M.H.

Regioselective [3 + 2] cycloaddition synthesis and theoretical calculations of new chromene-pyrazole hybrids: A DFT-based Parr Function, Fukui Function, local reactivity indexes, and MEP analysis

(2022) *Journal of Molecular Structure*, 1267, art. no. 133583. Cited 14 times.

<https://www.journals.elsevier.com/journal-of-molecular-structure>  
doi: 10.1016/j.molstruc.2022.133583

[View at Publisher](#)

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