

Science and Engineering *In Silico*

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Improvements in high-performance computing facilities in addition to improvements of theoretical aspects have led both of science and engineering to be investigated *in silico*. Within this new environment besides already available *in vitro* and *in vivo* media, the mechanisms of designing prior to perform any experiments have been tremendously generated.¹ Using computers, theories and mathematics algorithms have provided new facility for researchers in all fields of science and engineering to investigate their ideas in the silicon-based processors of computers.² Upon different expectations, specific software packages have been evaluated in both of open and closed sources. Programmers have also provided several coding routs to be combined for solving a problem of research tasks. In addition to molecular modeling, industry could employ *in silico* based engineering for managing the processes of productions. No-human fully digital industries are constructed based on computer-aided design and manufacturing from tiny sensors to huge Boeing 777s. Therefore, it seems that the claim of “The Near Future is Digital” is going to be applicable for different research areas and industries properly.³ Cyber science and engineering are crucial essentials for the 4th phase of industrial revolution to yield “Smart Factories”.⁴

Amazingly, the machines will work together and a human can monitor several of them by only a cell phone from home or any other convenient place.⁵ In the case of living systems, novel medicinal and pharmaceutical industries are trying to improve the life quality by initiating modern medical therapies including novel pharmaceutical compounds. In the cell-based therapy, molecular level machines are needed to enter inside the body to reach the correct cells for doing specific activities. So, a programmable machine should do such expectations under control of smart *in silico* based technologies. Targeted drug delivery systems are conducted by simulating living body and monitoring what happens inside it.^{6,7} It could be carefully recognized which drug could be properly useful for inhibiting an over-activated enzyme to prevent a disease growth. From the first drug design to the last clinical trials so many details could be very much carefully investigated by the *in silico* insights. Moreover, complicated aspects of nanotechnology have been also improved based on employing *in silico* methods for their characteristic investigations.⁸⁻¹⁴ As a conclusion, it seems to be the time to include the *in silico* insights in our classical and modern science and engineering areas to reach unavoidable Digital Future.

References

1. Geris L, Lambrechts T, Carlier A, Papantoniou I. The future is digital: *in silico* tissue engineering. *Cur. Opin. Biomed. Eng.* 2018;6:92-98.
2. Kazmi SR, Jun R, Yu MS, Jung C, Na D. *In silico* approaches and tools for the prediction of drug metabolism and fate: A review. *Comput. Biol. Med.* 2019;106:54-64.
3. McGann J. The future is digital. *J. Victor. Cult.* 2008;13:80-88.
4. Barbosa GF, Shiki SB, Savazzi JO. Digitalization of a standard robot arm toward 4th industrial revolution. *Int. J. Adv. Manufact. Technol.* 2019;105:2707-2720.
5. Mirzaei M. Lab-in-Silico. *Adv. J. Chem. B* 2020;2:1-2.
6. Samadi Z, Mirzaei M, Hadipour NL, Khorami SA. Density functional calculations of oxygen, nitrogen and hydrogen electric field gradient and chemical shielding tensors to study hydrogen bonding properties of peptide group (OC-NH) in crystalline acetamide. *J. Mol. Graph. Model.* 2008;26:977-981.
7. Behzadi H, Hadipour NL, Mirzaei M. A density functional study of 17O, 14N and 2H electric field gradient tensors in the real crystalline structure of α -glycine. *Biophys. Chem.* 2007;125:179-183.

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8. Mirzaei M. Effects of carbon nanotubes on properties of the fluorouracil anticancer drug: DFT studies of a CNT-fluorouracil compound. *Int. J. Nano Dimen.* 2013;3:175-179.
9. Mirzaei M, Yousefi M. Computational studies of the purine-functionalized graphene sheets. *Superlat. Microstruct.* 2012;52:612-617.
10. Mirzaei M, Mirzaei M. The C-doped AIP nanotubes: A computational study. *Solid State Sci.* 2011;13:244-250.
11. Mirzaei M. Density functional study of defects in boron nitride nanotubes. *Z. Phys. Chem.* 2009;223:815-823.
12. Mirzaei M, Mirzaei M. The B-doped SiC nanotubes: A computational study. *J. Mol. Struct. THEOCHEM.* 2010;953:134-138.
13. Mirzaei M, Hadipour NL, Seif A, Giahhi M. Density functional study of zigzag BN nanotubes with equivalent ends. *Physica E* 2008;40:3060-3063.
14. Mirzaei M, Meskinfam M. Computational studies of effects of tubular lengths on the NMR properties of pristine and carbon decorated boron phosphide nanotubes. *Solid State Sci.* 2011;13:1926-1930.

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