

it is required to gather enormous experimental data to improve the models of adequately high accuracies.

Finally, considering all attempts have been made in this intriguing field of study, it is anticipated that the MD simulations find their way in the near future to the clinics by predicting the effectiveness of various DDSs. This is reasonable as the MD computational methods consider very much larger systems than ab initio and DFT methods. Moreover, a combination of ab initio, DFT and MD simulations can be used to predict various physicochemical properties of the designed drug carriers. This allows selection of the most suitable DDS before its trial on the patients. Hence the MD simulations can reveal promising clinical applications in future.

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REFERENCES

- [1] D. Ailincăi, G. Gavril, L. Marin, Polyvinyl alcohol boric acid—a promising tool for the development of sustained release drug delivery systems, *Mater. Sci. Eng. C* 107 (2020) 110316.
- [2] M. Akbarian, S. Mahjoub, S.M. Elahi, E. Zabihi, H. Tashakkorian, Green synthesis, formulation and biological evaluation of a novel ZnO nanocarrier loaded with paclitaxel as drug delivery system on MCF-7 cell line, *Colloids Surf. B: Biointerfaces* 186 (2020) 110686.
- [3] G.F.B. Almeida, M.R. Cardoso, D.C. Zancanela, L. L. Bernardes, A.M.Q. Norberto, N.R. Barros, C. G. Paulino, A.L.D. Chagas, R.D. Herculano, C. R. Mendonça, Controlled drug delivery system by fs-laser micromachined biocompatible rubber latex membranes, *Appl. Surf. Sci.* 506 (2020) 144762.
- [4] Z. Shariatinia, Carboxymethyl chitosan: properties and biomedical applications, *Int. J. Biol. Macromol.* 120 (2018) 1406–1419.
- [5] Z. Shariatinia, Pharmaceutical applications of chitosan, *Adv. Colloid Interf. Sci.* 263 (2019) 131–194.
- [6] J. Bannow, Y. Yorulmaz, K. Löbmann, A. Müllertz, T. Rades, Improving the drug load and in vitro performance of supersaturated self-nanoemulsifying drug delivery systems (super-SNEDDS) using polymeric precipitation inhibitors, *Int. J. Pharm.* 575 (2020) 118960.
- [7] Q. Duan, L. Ma, B. Zhang, Y. Zhang, X. Li, T. Wang, W. Zhang, Y. Li, S. Sang, Construction and application of targeted drug delivery system based on hyaluronic acid and heparin functionalised carbon dots, *Colloids Surf. B: Biointerfaces* 188 (2020) 110768.
- [8] Z. Shariatinia, Chapter 2. Pharmaceutical applications of natural polysaccharides, in: M.S. Hasnain, A.K. Nayak (Eds.), *Natural Polysaccharides in Drug Delivery and Biomedical Applications*, Academic Press, 2019, pp. 15–57.
- [9] Z. Shariatinia, A. Barzegari, Chapter 22. Polysaccharide hydrogel films/membranes for transdermal delivery of therapeutics, in: S. Maiti, S. Jana (Eds.), *Polysaccharide Carriers for Drug Delivery*, Woodhead Publishing, 2019, pp. 639–684.
- [10] M.-R. Ki, J.K. Kim, S.H. Kim, T.K.M. Nguyen, K.H. Kim, S. P. Pack, Compartment-restricted and rate-controlled dual drug delivery system using a biosilica-enveloped ferritin cage, *J. Ind. Eng. Chem.* 81 (2020) 367–374.
- [11] Y. Fazli, Z. Shariatinia, Controlled release of cefazolin sodium antibiotic drug from electrospun chitosan-polyethylene oxide nanofibrous Mats, *Mater. Sci. Eng. C* 71 (2017) 641–652.
- [12] Y. Fazli, Z. Shariatinia, I. Kohsari, A. Azadmehr, S. M. Pourmortazavi, A novel chitosan-polyethylene oxide nanofibrous mat designed for controlled co-release of hydrocortisone and imipenem/cilastatin drugs, *Int. J. Pharm.* 513 (2016) 636–647.
- [13] A. Mazloom-Jalali, Z. Shariatinia, I.A. Tamai, S. R. Pakzad, J. Malakootikhah, Fabrication of chitosan-polyethylene glycol nanocomposite films containing ZIF-8 nanoparticles for application as wound dressing materials, *Int. J. Biol. Macromol.* 153 (2020) 421–432.
- [14] I. Kohsari, Z. Shariatinia, S.M. Pourmortazavi, Antibacterial electrospun chitosan-polyethylene oxide nanocomposite mats containing ZIF-8 nanoparticles, *Int. J. Biol. Macromol.* 91 (2016) 778–788.
- [15] I. Kohsari, Z. Shariatinia, S.M. Pourmortazavi, Antibacterial electrospun chitosan-polyethylene oxide nanocomposite mats containing bioactive silver nanoparticles, *Carbohydr. Polym.* 140 (2016) 287–298.
- [16] H. Liu, J. Liu, X. Xie, X. Li, Development of photo-magnetic drug delivery system by facile-designed dual stimuli-responsive modified biopolymeric chitosan capped nano-vesicle to improve efficiency in the anesthetic effect and its biological investigations, *J. Photochem. Photobiol. B Biol.* 202 (2020) 111716.
- [17] A. Luaces-Rodríguez, C. Mondelo-García, I. Zorra-Ferro, M. González-Barcia, P. Aguiar, A. Fernández-Ferreiro, F.J. Otero-Espinar, Intravitreal anti-VEGF drug delivery systems for age-related macular degeneration, *Int. J. Pharm.* 573 (2020) 118767.
- [18] Z. Nikfar, Z. Shariatinia, The RGD tripeptide anticancer drug carrier: DFT computations and molecular dynamics simulations, *J. Mol. Liq.* 281 (2019) 565–583.
- [19] Z. Nikfar, Z. Shariatinia, DFT computational study on the phosphate functionalized SWCNTs as efficient drug delivery systems for anti-osteoporosis zolendronate and risedronate drugs, *Phys. E* 91 (2017) 41–59.