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Digital twin to support the design and manufacture of functional nanoparticles with applications in biomedicine

We are standing at a unique crossroads in the fabrication of nanoparticles in-house [1-6] and AI algorithms. A decade from now, we have seen computational power explode, giving us the tools to dream up new biocompatible materials as novel drugs and treatments, designed faster than ever before. However, in the high-stakes world of nanomedicine, simply having a 'black-box answer' from AI isn't enough, it must be understandable. We don't just need algorithms that predict; we need algorithms that are interpretable. Our project mission is to bridge the gap between complex Deep Learning [7] and human understanding with the help of computer molecular simulations. In this poster, I will present the various experimental, as well as computational efforts performed by two groups at the material science's institute of Barcelona. Both synergetically working in three different project stages to achieve this ambitious objective which motivates us, namely, (i) the establishment of a 'global'database infrastructure for the systematic storage of experimental results; (ii) creation of complementary data from molecular dynamics simulation models to be used together with experimental data to improve the predictive power of AI models; and (iii) the development of statistical and artificial intelligence models capable of extracting properties and physico-chemical characteristics from our dataset of macromolecular structures. References [1] I. Cabrera et al., Nano Lett. 13(8), 3766–3774 (2013) [2] J. Tomsen et al., ACS Appl. Mater. Interfaces 13 (7), 7825–7838 (2021) [3] L. Ferrer-Tasies et al., Adv. Therapeutics 4(6) 2000260 (2021) [4] M. Martínez-Miguel et al., ACS Appl. Mater. Interfaces 14(42), 48179–48193 (2022) [5] J. Morlà et al., Chem. Mater. 34 (19), 8517–8527 (2022) [6] A. Boloix et al., Small 18(3) 2101959 (2022) [7] U. Pratiush, ⋯, H.V. Guzman, et al.,S.V. Kalinin, Mic-hackathon 2024: Hackathon on Machine Learning for Electron and Scanning Probe Microscopy, Mach. Learn.: Sci. Technol. 2025, 6, 040701

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