

MBN Explorer and Studio case studies with irradiation driven molecular dynamics

A.V. Solov'yov

MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany

solovyov@mbnresearch.com

MesoBioNano (MBN) Explorer [1] is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics developed by MBN Research Center. It has many unique features and a wide range of applications in Physics, Chemistry, Biology, Materials Science, and Industries. A broad variety of algorithms and interatomic potentials implemented in the program allows simulations of structure and dynamics of a very broad range of systems with the sizes from the atomic up to the mesoscopic scales, see [2] and references therein. MesoBioNano (MBN) Studio is a special multi-task software toolkit with graphical user interface developed for MBN Explorer [3] to facilitate setting up and starting MBN Explorer calculations, monitoring their progress and examining the calculation results.

The talk will give an overview of the main features of the packages and will highlight a number of recent case studies devoted to irradiation driven molecular dynamics [3,4,5].

References

[1] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, and A.V. Solov'yov, *MesoBioNano Explorer - a universal program for multiscale computer simulations of complex molecular structure and dynamics*, J. Comput. Chem. **33**, 2412 (2012); www.mbnresearch.com; wikipedia.org/wiki/MBN_Explorer

[2] I.A. Solov'yov, A.V. Korol, A.V. Solov'yov, *Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer*, Springer International Publishing AG (2017), Cham, Switzerland, 451 pp., ISBN: 978-3-319-56085-4 (hardcover), ISBN: 978-3-319-56087-8 (e-book); I.A. Solov'yov, G.B. Sushko, A.V. Solov'yov, *MBN Explorer Users' Guide: Version 3.0*, Verlag: CreateSpace Independent Publishing Platform (2017), 264 pp., ISBN: 978-1-975-63904-4; I.A. Solov'yov, G.B. Sushko, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, *MBN Explorer and MBN Studio Tutorials: Version 3.0*, Verlag: CreateSpace Independent Publishing Platform (2017), 288 pp., ISBN: 978-1-976-46092-0

[3] G.B. Sushko, I.A. Solov'yov, and A.V. Solov'yov, *Modeling MesoBioNano systems with MBN Studio made easy*, J. Mol. Graph. Model. **88**, 247 (2019)

[4] G.B. Sushko, I.A. Solov'yov, and A.V. Solov'yov, *Molecular dynamics for irradiation driven chemistry: application to the FEBID process*, Eur. Phys. J. **D70**, 217 (2016)

[5] A.V. Verkhovtsev, A.V. Korol, and A.V. Solov'yov, *Classical molecular dynamics simulations of fusion and fragmentation in fullerene-fullerene collisions*, Eur. Phys. J. D, vol. 71, 212 (2017)