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Toward Hands-on Molecular Design and Testing Enabled by Interactive VR Simulation

Gutmann Gregory Spence[1,3]
gutmann.g.aa@m.titech.ac.jp

Zhang Yuhui[1,3]
zhang.y.av@m.titech.ac.jp

Hirotada Kondo[2]
kondo@vraide.jp

Akihiko Konagaya[3]
konagaya@molecular-robot.com

[1] Tokyo Institute of Technology, School of Computing
[2] Kansai University, Chemistry and Materials Engineering
[3] Molecular Robot Research Institute, Co., Ltd.

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Works in molecular and nanoscale research and engineering continue to be more common as the desire for better drugs, nanoscale machines, and materials are constant. However, the process of designing at the nano-scale is complicated by the fact that we cannot see or interact with target molecular objects directly due to their sizes. As a solution to this, we are proposing a method that will enable hands-on design and testing of nanoscale structures and systems. We are proposing an interactive VR simulation system that enables users to dive into the molecular world and interact with biomolecules at the nanoscale, as well as simulate with conventional MD equations. It is feasible that we could load atomic structures, probe their dynamics in VR, reposition them in solvent, simulate with conventional equations, and then probe the dynamics again to see the changes in the system. This would enable researchers to quickly set up experiments and obtain results in a hands-on manner, in contrast to time-consuming data entry, or relying on testing large sets of random initial conditions to find possible solutions.

By combining an interactive VR environment and molecular dynamics simulation, we believe our proposed work will be able to offer greater insight into the molecular world and enable a greater degree of control over the setup of virtual experiments, enabling users to analyze and understand the molecular world in greater detail as it floats in front of them in VR.

[1] Gregory Gutmann, Ryuzo Azuma, Akihiko Konagaya: A Virtual Reality Computational Platform Dedicated for the Emergence of Global Dynamics in a Massive Swarm of Objects, *J. of the Imaging Society of Japan*, **2018**, 57(6), 647-653.