

**Building and Assessing a Web-based, Accessible, Three-Dimensional
Modeling Tool to allow High School Students to Explore Molecular Structure,
Intermolecular Interactions, and Molecular Dynamics Simulations**

by

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Abstract

Chemical bonding is the basis of many fundamental ideas in chemistry but is a difficult concept to teach due to common simplifications in textbooks, inaccurate or confusing terminology, and inadequate traditional testing methods to assess student understanding. The EMMAs (Exploring Molecular Modeling Activities) are a series of educational activities designed by *Kotsalidis et al.* to teach high school chemistry students about noncovalent bonding through case studies and exploratory exercises using the 3D molecular visualization tool VMD (Visual Molecular Dynamics). A prior study on the EMMAs found that the activities improved student understanding of noncovalent interactions. However, VMD is not available on Chromebooks, the most commonly-used personal computers used by high school students, and it also requires installation. Thus, my thesis builds and evaluates a web-based molecular visualization interface that implements the EMMAs, which will make these activities accessible to more students. We found that the web-based interface, despite some performance lags and potential to improve usability, was easier to use than VMD and other molecular visualization tools. Common feedback received involved requests to improve performance of rotation and loading, to add additional features to improve usability, and to improve the design to improve learnability. Future directions include incorporating focus group feedback before testing the web-based interface with the EMMAs at Wellesley High School in order to enable a more direct comparison between the original EMMAs study using VMD and the EMMAs with the web-based interface.

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