

## MOE Overview

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MOE, the Molecular Operating Environment, is a computational chemistry platform that integrates applications for drug discovery and life science research. A key feature of MOE is that it integrates not only the application execution environment, but also the molecular structure database function and a development environment. MOE offers various applications, including docking simulation, molecular dynamics simulation, SAR analysis, library analysis, fragment drug discovery, pharmacophore analysis, protein modeling, protein mutation analysis and so on. These applications can support a wide range of molecular design needs. MOE adopts its original database file format, MDB (Molecular Database), for effectively processing huge data used in computational chemistry. It can be accessed in high speed through the spreadsheet-like user interface. As the development environment, MOE is equipped with the Scientific Vector Language (SVL), a computer language developed for scientific computing. Almost all MOE applications are written in SVL, allowing users to check each application at the source code level. Moreover, users can freely customize and develop new applications using SVL. Thus, MOE can flexibly meet the various needs of researchers. In this presentation, I will give an overview of MOE and introduce some of many add-on programs that we have developed.