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Culgi: The Chemistry Unified Language Interface, a practical tool for general purpose chemical modeling.

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Computer modeling is a valuable tool for efficient formulation development of so-called soft materials in such diverse industries as chemicals, petroleum, pharmaceuticals, automotive, aerospace, and home & personal care. Integrating modeling activities into the R&D process increases the rate at which new products can be brought to market. A number of modeling techniques, ranging from atomistic to field based mesoscopic models, to statistical methods are used to solve various problems in the research process. Culgi (Chemistry Unified Language Interface) aims to integrate all relevant chemical modeling tools in one common platform. Modeling techniques include quantum, molecular, mesoscopic modeling and statistical methods such as Quantitative Structure Activity Relations. The library is designed from first principles up, in a C++ set of classes and functions, that can fully be controlled by common scripting languages such as tcl and python, but also by the powerful scripting editing tools from Culgi's Graphical Programming Environment. The novel design implies that the user, that is the industrial engineer or computational chemist, can develop proprietary applications easily. Thus, the library interfaces neatly between the expert software developer and application scientist. We discuss a few realistic business cases, including all aspects of successful industrial multiscale modeling, such as the importance of strong commitment to IT services and scientific consulting, as well as demonstration of dedicated workflows or script technology. Examples include drug delivery, commodity (polymer blends) and glues. An in-depth analysis of micro-emulsion design in the context of chemical oil recovery (in collaboration with Shell) is discussed in a separate presentation at this conference. Culgi is sponsored by several EU projects (Multimatdesign – Polymer Membranes, Selfmem – Polymer Membranes, Nanomodel – Nanocomposites, Biomimetic – Adhesives), Dutch government projects (Space Research, Biosolar Cells, and Microfluidics), and leading European, US and Japanese companies from a wide variety of industrial sectors. Culgi has development and support offices in Europe, China and USA, and representatives in Japan.

Keywords: computational chemistry, multiscale modeling, quantum; molecular, mesoscopic modeling.