

A Simple Language for Conversing between Diverse Applications

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Applications written for use in materials science research, 2D and 3D chemistry feature specialised chemistry engines that support chemical representation requirements unique to each individual domain. The use of different chemical engines presents a challenge when a user needs to communicate chemical data between applications without suffering from a loss of information. In this presentation, we will discuss how Accelrys has solved the problem of transferring chemical data between such applications in a lossless manner via the development of an extensible XML-based chemistry data format.