Siemens Competition
Math : Science : Technology
Regional Finalist

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High School: A&M Consolidated High School
Mentor: Professor Dr. Tapas Kar
Project Title: *Generalized Interatomic Two-Body Potential-Energy Functions* (Physics)

Since 1918, more than 110 two-body potential-energy functions (TBPEFs) have been reported. The piecewise TBPEF form lacks a certain uniqueness and is cumbersome for application, while the other ones often lose the validity for either small or large inter-nuclear distances. Is it possible to construct a unique TBPEF form that is able to describe accurately the entire potentials of the diatomic systems? The question has puzzled scientists for over 40 years. This report shows a possibility to achieve such a function. Explicitly, based on a three-parameter molecular orbital-type TBPEF, a generalized TBPEF is proposed and demonstrated to be able to describe accurately the entire potentials of the ground or metastable states of a wide variety of diatomic systems. Considering the limited increment of this new TBPEF in complexity as compared to the three-parameter TBPEF, the improvement in accuracy and the extension in applicability are impressive. Also, it is demonstrated that the new TBPEF is competitive to other TBPEFs for the benchmark test examples. The new TBPEF is likely to see future use, for example, in the geometry optimization or dynamics study of large atomic clusters, biomolecules, and others .