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High precision variational calculations of few-electron atoms[1]
SERGIY BUBIN, Nazarbayev University — High precision calculations of energy levels and other properties of small atoms and ions have been a subject of fruitful interplay between the experiment and theory. However, most calculation of spectroscopic accuracy, until recently, have been possible only for two- and three-electron systems. In this talk I will report on progress toward performing high accuracy calculations of larger atomic systems (up to four-six electrons). The results of benchmark quality are attainable with the use of variational expansions in terms of all-particle explicitly correlated Gaussians, whose nonlinear variational parameters are extensively optimized. I will demonstrate what level of accuracy is available today for few-electron atoms and discuss the issues that must be overcome in order to extend the capability of the method to even larger systems.

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