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Towards accurate predictions of clock transitions in highly charged ions with complex electronic structure CHARLES CHEUNG, MARIANNA SAFRONOVA, SERGEY PORSEV, University of Delaware, MIKHAIL KOZLOV, Petersburg Nuclear Physics Institute of NRC, ILYA TUPITSYN, St. Petersburg State University — Highly charged ions such as Ir^{17+} are attractive candidates for the development of novel atomic clocks with high sensitivity to the variation of the fine-structure constant. The clock transitions are weak and are difficult to identity without accurate theoretical predictions. The cases of Ir^{16+} and Ir^{17+} are particularly difficult due to atomic configurations with holes in the $4f$ shell leading to a very large number of configurations that have to be included within the framework of the configuration interaction (CI) approach. In this work, we developed strategies to identify most important configurations using valence perturbation theory (PT) which can be used to improve and optimize the CI valence space. A parallel version of the code has also been developed, allowing us to perform computations with factor of a 100 larger CI spaces than before within a reasonable computational time. We find that including large number of configurations is necessary for accurate calculations and demonstrate saturation of the CI space for the 15-valent Ir^{16+} and 14-valent Ir^{17+} ions using this method. We calculate low-lying energy levels and transition rates relevant to atomic clock development and compare the results with other values.

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