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# Ionization potential and electron affinity of element 119

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The discovery and study of new chemical elements has been one of the most important areas of physical research for a long time [1]. Currently, the heaviest synthesized superheavy element (SHE) is oganesson (Og, Z = 118) [2], which completes the seventh period of the periodic table. The lightest of the experimentally undefined elements is eka-francium, also known as ununennium (Uue, Z = 119). An attempt to synthesize the 119th element was made at the Helmholtz Centre for Heavy Ion Research (GSI) [3]. For several years, the experiment has been conducted at the RIKEN Nishina Center [4]. Plans to synthesize eka-francium are being made by scientists from the Joint Institute for Nuclear Research (JINR) [5] and the Institute of Modern Physics of the Chinese Academy of Sciences (IMP) [6].

The interest in studying properties of superheavy elements is largely driven by the desire to determine the limits of applicability of the periodic law, according to which elements in the same group have similar properties. However, it is not uncommon for some properties of superheavy elements to differ significantly from those of their lighter homologs. The difference in the electronic structure of superheavy elements from that of their lighter homologs is caused, on the one hand, by the increasing influence of relativistic effects associated with the increasing nuclear charge, and on the other hand, by the influence of electronic correlations associated with the increasing number of electrons.

This work presents the optimization of the basis set for eka-francium, obtained in [7] using the p-GCDF method. With its help, the values of the ionization potential and electron affinity for this element were calculated within the framework of the coupled-cluster method. Optimization of the basis set significantly affects ionization potential and electron affinity of the 119th element: both values increase by approximately 0.15 eV. This is particularly noticeable for the electron affinity, with a change of around 60% of its value calculated using the unoptimized basis set. The calculations were carried out using the DIRAC [8] and EXP-T [9] software packages.

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1. Oganessian Y.T., Utyonkov V.K. Super-heavy element research // Reports on Progress in Physics. 2015. V. 78, No. 3. P. 036301.
2. Oganessian Y.T. et al. Synthesis of the isotopes of elements 118 and 116 in the $^{249}$Cf and $^{245}$Cm+$^{48}$Ca fusion reactions // Physical Review C—Nuclear Physics. 2006. V. 74. No. 4. P. 044602.
3. Khuyagbaatar J. et al. Search for elements 119 and 120 // Physical Review C. 2020. V. 102. No. 6. P. 064602.
4. Sakai H. et al. Facility upgrade for superheavy-element research at RIKEN // The European Physical Journal A. 2022. V. 58. No. 12. P. 238.
5. Oganessian Y.T. et al. First experiment at the Super Heavy Element Factory: High cross section of $^{288}$Mc in the $^{243}$Am+$^{48}$Ca reaction and identification of the new isotope $^{264}$Lr // Physical Review C. 2022. V. 106. No. 3. P. L031301.
6. Gan Z.G. et al. Results and perspectives for study of heavy and super-heavy nuclei and elements at IMP/CAS // The European Physical Journal A. 2022. V. 58. No. 8. P. 158.
7. Miranda P.S. et al. Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F) // Journal of the Brazilian Chemical Society. 2012. V. 23. P. 1104-1113.
8. Saue T. et al. The DIRAC code for relativistic molecular calculations // The Journal of Chemical Physics. 2020. V. 152. No. 20.
9. Oleynichenko A.V., Zaitsevskii A., Eliav E. Towards high performance relativistic electronic structure modelling: The EXP-T program package // Russian Supercomputing Days. – Cham: Springer International Publishing, 2020. P. 375-386.