Model of single-electron transistor based on prismanes

Ainur Duisenova[1*], Daulet Sergeyev[2]
[1]*K. Zhubanov Aktobe Regional University, 34A Moldagulova avenue, 030000 Aktobe, Kazakhstan*
[2] *T. Begeldinov Aktobe Aviation Institute, 39 Moldagulova avenue, 030012 Aktobe, Kazakhstan*
*E-mail: ainura_duisenova@mail.ru

In recent years, the effect of correlated tunneling of single electrons has been used to solve the further reduction in the size of electronic elements. The essence of this effect is the Coulomb blockade of electron transport and orderly motion of elementary charges, arising due to their interaction by means of an electric field. This led to the birth of single-electronics, the "core" of which is electronic devices based on single molecules. In this work, within the framework of density functional theory, the transport properties of a single-electron transistor (SET) based on C12H12, C12F12, C18H12, C18F12 prismanes are model investigated. The optimization of prismane molecules was carried out using the exchange-correlation functional of the generalized gradient approximation (GGA), which allows to describe such structures most accurately. The electrostatic difference potential, molecular energy spectrum, and total energy SET are calculated on the basis of prismanes. It is shown that the area of Coulomb diamond SETs based on prismane with passivated hydrogen atoms (C12H12) is significantly larger than others, also significantly decreases when a hexagonal ring (C18H12) is added in the central part. It is revealed that the area of the Coulomb diamond SET based on the prismane passivated with fluorine atoms (C12F12) is smaller, but when a hexagonal ring (C18F12) is added in the central part, it increases noticeably. The values of gate voltage for opening prismane transistors with a minimum source-drain VSD voltage are determined. It is found that in transistors based on a – C12F12, b – C12F12 and c – C12F12 in the absence of gate voltage, current transport is blocked in the range of Source-Drain bias ±3.73V, ±4.28V and ±4.33V respectively, and in transistors based on a – C12H12, b – C12H12 and c – C12H12 in the absence of gate voltage, the Coulomb blockade acts within a small range of source-drain bias ±0.25V, ±0.35V and ±0.25V respectively. The conditions for switching transistors from the Coulomb blockade mode to the single-electron tunnelling mode are determined. The obtained results may be useful for the calculation of new types of SETs.

Acknowledgement
This research was supported by the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan (grant № AP08052562).