Precise calculation of the negative ions bond energies: perturbation theory with model zeroth approximation

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Within formally exact perturbation theory with ab initio model zeroth (density-functional theory, Tomas-Fermi approach) approximation [1] (modified variant of method [2]), it has been carried out the calculation of the energy characteristics of the heavy negative ions: Ge, Sn, Pb. The comprehensive correct procedures for account the electron correlation effects (the mutual screening and polarization inter-quasi-particle interaction of external quasi-particles, mass operator iterations) has been proposed and realized in the numeral calculation. A part of the results are obtained at first. In table there are presented some results of calculation of the electron affinity energies (EA) of some complex atoms (Si, Ge, Sn, Pb): A- values, recommended (on the basis of compilation) in ref. [3]; B- values, calculated in this work. Besides, it is important result: calculation results predict the existence of the stable negative ions of inert gas atoms: Kr* (EA=0,10eV) and Xe* (EA=0,14eV) in a low-lying excited state. At first such possibility has been predicted in ref. [3].

Ion	Configuration	Term	A (eV)	B (eV)
Si	$3p^3$	^4S	1,39	1,39
Si	$3p^3$	^2D	0,53	0,53
Si	$3p^3$	^2P	0,34	0,32
Ge	$4p^3$	^4S	1,20	1,16
Sn	$5p^3$	^4S	1,20	1,08
Pb	$6p^3$	^4S	0,37	0,41

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