

X-ray photoelectron and Auger electron transition energies of inorganic substances by DFT methods

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We have already investigated valence XPS, IR, and C13 NMR spectra of polymers using the model oligomers from DFT calculations [1]. In the present study, core-electron binding energies (CEBE)s and Auger electron spectra (AES) of alkali and alkali earth metal elements have been obtained by DFT calculations using the model molecules of the unit cell. For the calculations, we used unrestricted generalized transition-state (uGTS) method [2] in deMon DFT program [3] and B3LYP/6-31++G (d,p) level calculation in GAUSSIAN 09 software [4] to estimate the core-electron binding energies, respectively. Calculated CEBEs of the model molecules with uGTS method in Table 1 are in considerably good accordance with the experimental values. In the deMon DFT calculations, we used a reasonable method $\{I_{cjk} \cong [(CEBE, I_c^A) - (VIP, I_j) - (VIP^*, I_k^*) - WD]\}$; $[VIP^*; I_j, \text{ or } I_k^*]$, restricted diffusional ionization models (*rDI*, $q=+1$ (q is charge)), Auger *rDI*(A-*rDI*, $q=+2$), respectively], to evaluate transition energies of the AES. Calculated Auger electron transition energies for alkali and alkali earth metals correspond considerably well to experimental values of the substances.

Table 1. Core-electron binding energies of alkali and alkali earth metal

	Experimental	Calculated	
		uGTS (deMon DFT)	B3LYP/6-31G(d,p) (G9)
Lithium			
Li-metal (Li1s)	54.8±0.3 eV (ga: 64.4 eV),	64.576 eV	55.651eV
Sodium			
Na-metal(Na1s)	1072.0±0.3 (gas: 1079.1)	1090.984 eV	1048.206 eV
Potassium			
K-metal (K2s)	380 eV K-metal	377.148 eV	360.804 eV
K-metal (K2p)	294.5±0.4 eV(Gas:2p 300.7 eV)	311.475 eV	288.467 eV
Beryllium			
Be	111.8±0.3	129.112 eV	110.658 eV
Magnesium			
Mg 1s	1303 eV(Gas: 1311.2eV)	1311.625 eV	1274.574 eV
Mg 2s	89 eV(Gas 96.5eV)	88.232 eV	84.811 eV
Mg 2p	49.7±0.2eV (Gas 57.6 eV)	52.85 6eV	50.649 eV
Calcium			
Ca 2s	440eV, (Gas 447.5 eV)	430.579 eV	420.724 eV
(Ca2p)	346.4±0.5eV (Gas 356.0 eV)	359.478 eV	342.666 eV

References

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