

	姓名：李步通
	职称： 教授
	地址：贵阳市乌当区高新路 115 号
	Telephone: 0851-85816647
	E-mail: butong.lee@gmail.com
研究方向：	
功能材料设计与合成	
主要经历：	
2001/09–2006/06，吉林大学，理论化学研究所，博士 1997/09–2001/06，吉林大学，化学学院，学士	
主讲课程：	
结构化学，材料科学基础，物理化学实验，综合化学实验，计算机在化学中的应用，中学化学多媒体课件制作	
学术科研：	
<p>(1)) 项目：主持并结题省级课题两项，参加国家级课题五项</p> <p>(2) 发表主要论文：</p> <p>[1] LI B.-T., CHI W.-J., LI L.-L., Theoretical Calculation about the High Energy Density Molecules of Nitrate Ester Substitution Derivatives of Prismane, <i>Chinese J. Struct. Chem.</i>, 2016, 35, 1306—1312.</p> <p>[2] Chi W., Yan T., Li* B., Is 1-nitro-1-triazene a high energy density material?, <i>Journal of Molecular Modeling</i> 2014, 20, 2362-2367.</p> <p>[3] Yan T., Sun G., Chi W., Li* B., Wu H., Looking for high energy density compounds among polynitraminepurines, <i>Journal of Molecular Modeling</i>, 2013, 19, 3491-3499.</p> <p>[4] Yan T., Sun G., Chi W., Li L., Li* B., Wu H., Computational studies on thermodynamic properties, detonation properties and bond dissociation energies for polydifluoroaminopurine compounds, <i>Comptes Rendus Chimie</i> 2013, 16, 765-772.</p> <p>[5] Yan T., Chi W.-J., Bai J., Li L.-L., Li* B.-T., Wu H.-S., Computational studies on polynitropurines as potential high energy density materials, <i>Journal of Molecular Modeling</i>, 2013, 19, 2235-2242.</p> <p>[6] Chi W.-J., Li L.-L., Li* B.-T., Wu H.-S., Theoretical investigation on detonation performances and thermodynamic stabilities of the prismane derivatives, <i>Journal of Molecular Modeling</i>, 2013, 19, 1049-1057.</p>	

- [7] Chi W.-J., Li L.-L., Li* B.-T., Wu H.-S., Looking for high energy density compounds among polynitraminecubanes, *Journal of Molecular Modeling*, **2013**, *19*, 571-580.
- [8] Chi W., Li* B., Wu H., Density function theory study on energetic nitro-triaziridine derivatives, *Structura Chemica*, **2013**, *24*, 375-381.
- [9] Bai J., Chi W.-J., Li L.-L., Yan T., Wen X.-E., Li* B.-T., Wu H.-S., Ma F.-L., Quantum Chemical Study of Aminonitrocyclopentanesas Possible High Energy Density Materials (HEDMs), *Central European Journal of Energetic Materials*, **2013**, *10*, 467-478.
- [10] Li* B.-T., Li L.-L., Wu H.-S., Theoretical calculation about the valence and rydberg excited states of hydroger cyanide, *Journal of Computational Chemistry*, **2012**, *33*, 484-489.
- [11] Li B.-T., Wei Z.-Z., Wu H.-S., The valence and Rydberg excited states of CH₂: A theoretical exploration *Journal of Computational Chemistry*, **2012**, *33*, 2498-2503.
- [12] Chi W.-J., Li L.-L., Li* B.-T., Wu H.-S., Density functional calculations for a high energy density compound of formula C₆H_{6-n}(NO₂)_n, *Journal of Molecular Modeling*, **2012**, *18*, 3695-3704.
- [13] Chi W.-J., Li L.-L., Li* B.-T., Wu H.-S., Density functional study on the derivatives of purine, *Journal of Molecular Modeling*, **2012**, *18*, 3501-3506.
- [14] Chi W., Wang X., Li* B., Wu H., Theoretical investigation on the heats of formation and detonator performance in polydinitroaminocubanes, *Journal of Molecular Modeling*, **2012**, *18*, 4217-4223.
- [15] Chi W., Sun G., Liu T., Li* B., Wu H., Density functional theory calculations on the thermodynamic properties of polynitrosoprismanes, *Journal of Molecular Modeling*, **2012**, *18*, 4557-4563.
- [16] Chi W., Li L., Li* B., Wu H., Density functional calculation on a high energy density compound having the formula C₂O_{4-n}(NO₂)_n, *Structural Chemistry*, **2012**, *23*, 1837-1841.
- [17] Liu T., Li* B.-T., Theoretical study of the mechanics of the HCNO+OH reaction, *Journal of Shanxi Normal University (Natural Science Edition)*, **2009**, *23*, 58-63.
- [18] Wei Z.-Z., Li B.-T., Pan Q.-J., Zhang H.-X., Sun C.-C., Theoretical study on the low-lying electronic states and ionization spectra of fluorine nitrate, *Chemical Journal of Chinese Universities-Chinese*, **2008**, *29* 611-614
- [19] Wei Z.-Z., Li B.-T., Zhang H.-X., A theoretical investigation of the excited states of OCIO radical, cation, and anion using the CASSCF/CASPT2 method, *Journal of Computational Chemistry*, **2007**, *28*, 467-477.
- [20] Wei Z.-Z., Li B.-T., Pan Q.-J., Zhang H.-X., Sun C.-C., Accurate prediction of excited energy of rydberg states of OCIO and ab initio investigation of excited states of OCIO anion with a low energy, *Chemical Journal of Chinese Universities-Chinese*, **2007**, *28*, 2183-2186.
- [21] Li B.-T., Wei Z.-Z., Pan Q.-J., Zhang H.-X., Sun C.-C., CAS calculations for the ground- and excited-state properties of HSO radical, *Chemical Journal of Chinese Universities-Chinese*, **2007**, *28*, 1107-1109
- [22] Li B.-T., Wei Z.-Z., Pan Q.-J., Zhang H.-X., Sun C.-C., CAS calculations on the ground and low-lying excited states of ethylthio radical, cation and anion, *Chemical Journal of Chinese Universities-Chinese*, **2007**, *28*, 1972-1974.
- [23] Li B.T., Zhang J., Wu H.S., Sun G.D., Theoretical study on the mechanism of the NCO + HCNO reaction, *J Phys Chem A*, **2007**, *111*, 7211-7217.
- [24] Wei Z.-Z., Li B.-T., Pan Q.-J., Zhang H.-X., Sun C.-C., Theoretical studies on the low-lying excited states of ethyl bromide and its cation, *Chemical Journal of Chinese Universities-Chinese*, **2006**, *27*, 1903-1906.
- [25] Li B.-T., Wei Z.-Z., Pan Q.-J., Zhang H.-X., Sun C.-C., A theoretical study of excited states of HO₂ radical *Chemical Journal of Chinese Universities-Chinese*, **2006**, *27*, 2168-2170.
- [26] Li B.T., Wei Z.Z., Zhang H.X., Sun C.C., Theoretical studies on the low-lying electronic states of the HSC neutral radical and its cation, *J Phys Chem A*, **2006**, *110*, 10643-10650.

