Chinese Science Bulletin

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Springer

New development of concept of electronegativity

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The concept of electronegativity (EN), which was proposed by Pauling in 1932, is closely related to such properties of molecules as the polarizability, hardness (softness) and charge distribution, and is an important theoretical basis for judging the properties of substances. With the development of new materials and the increase of interdisciplinary cooperation, EN has been a basic atomic parameter which is widely used in the fields of chemistry, physics and materials science. The development of EN has involved three stages, atomic EN, ionic EN and bond EN. The ionic EN, which is the EN values of elements in different valence states by including the chemical environment of atoms, accurately describes various physical and chemical properties of ions and compounds. The bond EN is a bridge linking atomic EN and the properties of materials, which helps us to establish the quantitative correlation between macroscopic properties and microscopic electronic structures of materials. The concepts of ionic EN and bond EN broaden the scope of EN theory, and play important roles in the design of novel materials. This paper presents a detailed introduction of a new development of EN and its applications in materials research.

electronegativity, atoms, ions, chemical bonds, materials design

Electronegativity (EN) has long been one of the most important concepts in chemistry since it was proposed by Pauling in 1932. In his standard book, *The Nature of the Chemical Bond*, Pauling defined the EN as “the power of an atom in a molecule to attract electrons to itself”, and established the first quantitative EN scale on the basis of thermochemical data, which laid a workable foundation for the study of EN in the 20th century[1]. Because the Pauling EN was derived from heats of formation or, essentially, bond energies, the EN difference between two atoms reflects the strength of bonds, and moreover, there exists a quantitative correlation between EN and bond polarity. For more than 70 years, the concept of EN has been modified, expanded and debated, with such new concepts as ionic EN and bond EN emerging. These concepts enriched and extended EN theory, bringing EN study into a new development period. In recent years, functional materials design has been one of the most important research areas with the development of new materials. The complexity of well-developed quantum theory for solids limits its practical application, whereas EN has various practical benefits with regard to materials design. The concept of EN has been used to persuasively explain the geometries and properties of materials[2,3], such as superconductivity, photocatalytic activity, magnetic property and optical basicity[4–7]. In particular, EN based semiempirical models provide a useful guide in the prediction of the structures and properties of materials and for the further exploration of novel materials.

1 Atomic electronegativity

After Pauling’s pioneering work, extensive studies on EN have been carried out and numerous EN scales were proposed on the basis of various atomic parameters and

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Received June 2, 2008; accepted September 17, 2008
doi 10.1007/s11434-008-0578-9:

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Supported by the Program for New Century Excellent Talents in University (Grant No. NCET-05-0278) and Foundation for the Author of National Excellent Doctoral Dissertation of China (Grant No. 200322)

physical properties. The most representative scales are the Mulliken scale, Allred-Rochow scale, Sanderson scale, Allen scale, and Phillips scale. Mulliken defined EN as an average of ionization energy and electron affinity[8], which is an absolute EN scale based on experimental data, and also has a specific physical meaning. Pauling considered that Mulliken made an important contribution to the theory of the EN scale[9]. Allred and Rochow described EN as the electrostatic force at the covalent radius of an atom caused by its effective nuclear charge[10]. Sanderson regarded EN as a function of electron density, and he proposed the famous EN equalization principle, i.e., when two or more atoms initially different in EN combine, they adjust towards an equal intermediate EN in the compound. This principle was utilized to calculate the partial charge of atoms and the bond length in compounds[11]. Allen proposed that EN can be defined in terms of configuration energy, i.e., the average one-electron energy of the valence-shell electrons in the ground state free atom. He argued that EN is the third dimension of the periodic table[12]. Considering the screening effect of valence electrons on the nucleus, Phillips introduced an EN expression on the basis of the dielectric property of atoms[13]. In addition, Chen proposed an empirical expression of EN using the charge-radius ratio and some other parameters describing the radial distribution of the inner electrons[14]. Yuan defined EN as the ratio of the number of valence electrons to the covalent radius[15], which was later modified by Luo et al. and successfully applied to estimate the group parameters, heats of formation, bond dissociation energies and other properties of molecules[16]. Although these EN scales have different units, electrostatic potential has generally been accepted as the unit of EN since 1961[17]. It was not until 1978 that a milestone in the search for a rigorous theoretical definition of EN was reached by Parr et al.[18] Using density functional theory, they identified EN with the negative of the chemical potential, which is the derivative of the energy with respect to the number of electrons at a constant external potential. Parr's definition of EN provided solid theoretical basis for the Mulliken EN scale and Sanderson's EN equalization principle[18,19]. This absolute EN is a measure of the chemical reactivity of an atom, ion, radical, or molecule, which gives the direction of the electron flow and an estimate of the initial amount of electron density transferred, which, in turn, is related to energy barriers for reaction and to the strength of the coordinate bond formed.

On the other hand, the evaluation and testing of various EN scales have resulted in a wide range of research studies. Sproul evaluated 15 EN scales by the ionic, covalent, or metallic property for the 311 binary compounds, and proposed that a comprehensive EN scale would have the ablity to not only predict the nature of a chemical bond but also indicate the incorrect bond type specification[20]. Pearson suggested that different EN scales have different applications, and each scale is correct within its own area of application[21]. An effective scale of EN would adequately reflect the singularity and particularity of elements, and satisfactorily explain various physical and chemical properties of compounds. The Pauling scale is the first EN scale, which has been effectively used to predict bond polarity, solubility and the melting point of compounds. Therefore, it is the most widely used scale. The reliability of other EN scales is usually checked through comparison with the Pauling scale. Herein, we recommend the Pauling scale when using atomic EN (Table 1[22,23]).

2 Ionic electronegativity

For most EN scales, EN is always regarded as a property of isolated atoms, i.e., each element corresponds to a unique value. Actually, the EN of an element depends on its chemical environment, which involves different valence states, coordination numbers and even spin states within compounds. EN values are expected to be more accurate if the effect of the environment is taken into account[24]. EN values of any ions may be selected by including their actual chemical environment, by which various physical and chemical properties of ions and compounds are most accurately described. In 1954, Sanderson proposed that the EN of elements is related to their valence states[25]. The EN of an element increases with increasing oxidation state and decreases with increasing radius, which is called EN in valence states, i.e., ionic EN. In 1982, Zhang proposed an empirical formula of ionic EN based on the effective nuclear charge of an ion and the covalent radius, which resulted in a table of EN of elements in valence states. Combined with the parameters characterizing the electrostatic force of ions, these EN values were utilized to quantitatively calculate the Lewis acid strength of metal cations[26]. In 1986, Sanderson computed the EN values of transition metals in different valence states using partial charges and bond

Table 1 Recommended values of atomic electronegativity

Period		IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA
I		H																
	χ_a	2.20																
II		Li	Be											B	C	N	O	F
	χ_a	0.98	1.57											2.04	2.55	3.04	3.44	3.98
III		Na	Mg											Al	Si	P	S	Cl
	χ_a	0.93	1.31											1.61	1.90	2.19	2.58	3.16
IV		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
	χ_a	0.82	1.00	1.36	1.54	1.63	1.66	1.55	1.83	1.88	1.91	1.90	1.65	1.81	2.01	2.18	2.55	2.96
V		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
	χ_a	0.82	0.95	1.22	1.33	1.60	2.16	1.90	2.20	2.28	2.20	1.93	1.69	1.78	1.96	2.05	2.10	2.66
VI		Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
	χ_a	0.79	0.89	1.10	1.30	1.50	2.36	1.90	2.20	2.20	2.28	2.54	2.00	2.04	2.33	2.02	2.00	2.20
VII		Fr	Ra	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
	χ_a	0.70	0.90	1.12	1.13	1.14		1.17	1.18	1.20		1.22	1.23	1.24	1.25		1.27	

energies, which was used to explain the stability principle of some transition metal compounds[27].

Recently, we proposed a new ionic EN model on the basis of effective ionic potential[28]. In the compound, the cations are surrounded by a certain number of anions to maintain their stability, and anions are also stabilized in the electrostatic potentials of cations. Therefore, the attractive ability of an ion can be expressed as the electrostatic potential at the boundary of the ion caused by its effective nuclear charge

$$\varphi_i = Z^* / r_i , \tag{1}$$

where Z^* is the effective nuclear charge, and r_i is the ionic radius. According to the Slater rule, for a cation M^{j+}, the jth ionization energy can be expressed as $I_j = RZ^{*2}/n^{*2}$ [26], where n^* is the effective principal quantum number, and R = 13.6 eV is the Rydberg constant. Therefore, the effective nuclear charge of the cation can be expressed as $Z^* = n^*(I_j/R)^{1/2}$. By substituting this equation into eq. (1), the effective ionic potential can be obtained. In order to obtain widely accepted values, we plotted the Pauling EN against the effective ionic potential φ_i, with the expression of the ionic EN model determined through a linear regression

$$\chi_i = 0.105 \frac{n^* (I_j / R)^{1/2}}{r_i} + 0.863 , \tag{2}$$

where 0.105 and 0.863 are fitting constants. Taking Fe^{2+} as an example, I_j is the second ionization energy I_2 of iron, and r_i is the ionic radius of Fe^{2+}. According to Eq.(2), we determined the EN values of 82 elements in the periodic table with different valence states, coordination numbers and spin states. Due to the detailed consideration of the actual chemical environment of ions, this scale was well applied to the estimation of such useful physical and chemical parameters as the Lewis acid strength and the hydration free energy of cations[28]. It was found that there exists a linear relationship between the hydration free energy ΔG_{hyd} (the hexa-hydrated complex $M(H_2O)_6^{2+}$) of divalent cations M^{2+} for the first transition series and the EN of the cations, i.e., $\Delta G_{\text{hyd}}(\text{kcal}/\text{mol}) = -533.20\chi_i + 253.66$ (Because water is typically a weak-field ligand, we chose EN values of M^{2+} in the high-spin state). Figure 1 shows that the predicted values agree well with the calculated values from the quantum chemistry method[29].

This EN scale is useful for exploring the structure-property relationship of materials. Rare earth lumines-

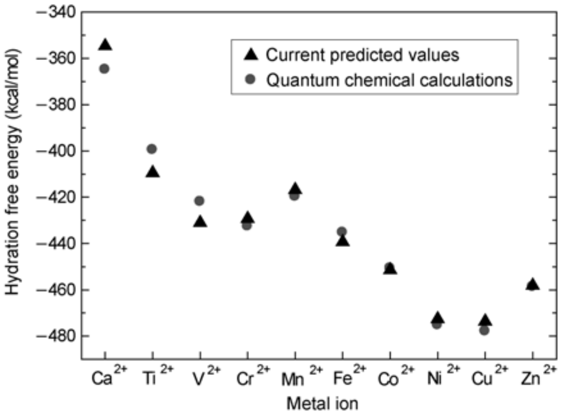

Figure 1 Comparison of predicted hydration free energies with quantum chemical calculated values (data are taken from Ref. [29]) for divalent cations of the first transition series.

cent materials have been intensively investigated due to their practical applications in such fields as display, lasers and medicine. The valence change of rare earth ions is a process of gaining or releasing valence electrons, and the energy of its charge-transfer band is also a measure of the ability of rare earth central ions to attract electrons from ligands. Therefore, both the valence change and the charge-transfer energy of rare earth ions are related to their EN[30]. However, the available EN values of lanthanide elements are either scarce or does not sufficiently reflect the different electron-attracting abilities of the lanthanide ions, which has limited the applications of EN in the research of rare earth materials. Figure 2 indicates that the trend of change for the charge-transfer energy of trivalent lanthanides (Ln^{3+}) in the YPO_4 host crystal is completely opposite to that of the EN of Ln^{3+} from La to Yb, both of which exhibit the Ln contraction and “gadolinium break” phenomena. A similar trend of change occurs when Ln^{3+} is in other host crystals such as CaF_2. This is because for a given host crystal, the larger the EN of Ln^{3+}, the stronger the electron-attracting power of the Ln^{3+} ion. Therefore, the electrons from the ligand will be more easily transferred to the Ln^{3+} impurity ion, which leads to the smaller charge-transfer energy of Ln^{3+}. Our EN values are thus useful for quantitatively estimating the charge-transfer energy of Ln^{3+}[31], which will be very helpful for investigating the novel rare earth luminescent materials. In addition, as an acceptor of electron pairs, the strength of a Lewis acid is measured by the electronattracting power of its central ions, therefore it is closely related to the EN of the ion. Brown and Luo systematically studied the relationship between Lewis acid strength and EN for main-group elements, and they found that Lewis acid strength increases with the increasing EN of the corresponding elements[32,33]. It is well-known that Ln^{3+} compounds are frequently employed as excellent Lewis acid catalysts in a wide range of important organic transformations. Figure 2 shows that the trend of our EN scale of Ln^{3+} ions is consistent with that of the average relative strength of Lewis acids for five Ln^{3+} compounds $[Ln(OTf)_2(L)_4]OTf$, i.e., Eu^{3+} and Yb^{3+} are higher than those of Gd^{3+} and Lu^{3+} (L = HMPA, TEPO, TMP, DMPU and DMSO, and the data for the relative Lewis acid strength are taken from ref. [34]). Figure 3 shows that there is a linear relationship between the Lewis acid strength of Ln^{3+} compounds and the EN of central ions, which further demonstrates the plausibility of our EN values for Ln^{3+}. We therefore conclude that our ionic EN scale may be the most reliable scale (Table 2[28]).

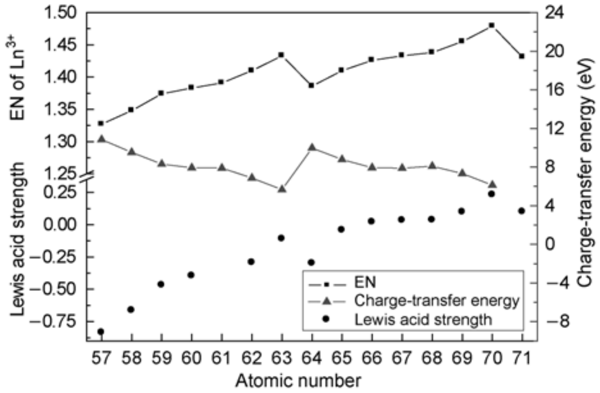

Figure 2 Change trends of EN of Ln^{3+}, average relative strength for five Lewis acids $[Ln(OTf)_2(L)_4]OTf$ (L = HMPA, TEPO, TMP, DMPU and DMSO) and charge-transfer energy of Ln^{3+} in YPO_4 crystals with the atomic number of Ln.

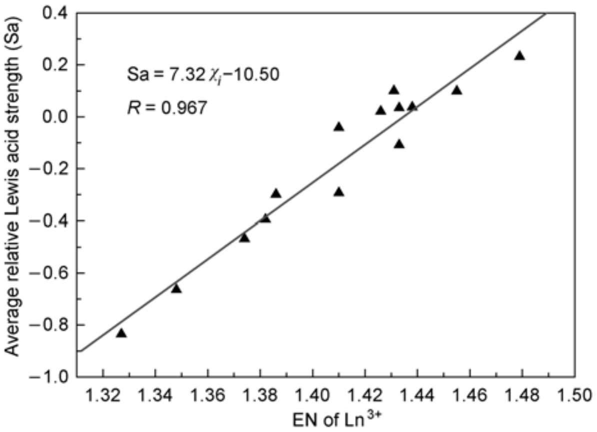

Figure 3 The relationship between the average relative strength for five Lewis acids $[Ln(OTf)_2(L)_4]OTf$ (L = HMPA, TEPO, TMP, DMPU and DMSO) and the EN of Ln^{3+}.

3 Bond electronegativity

Because the properties of molecules or crystals mainly depend on the nature of their constituent chemical bonds, similar to the transitions of other properties from atoms to bonds such as from atomic valence to bond valence, from atomic hardness (softness) to bond hardness (softness), and from atomic polarizability to bond polarizability, the definition of bond EN also more directly reflects the charge distribution of the bond, and more conveniently describes various physical and chemical properties of molecules or crystals. In 1963, Whitehead proposed the definition of orbital EN, and suggested that EN is a property of atomic orbitals. He defined the new term, bond EN, as being the EN of orbitals forming a

Table 2 Recommended values of ionic electronegativity*

Period		IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA
II		Li	Be											B	C	N	O	F
	χ_i	(1)1.009	(2)1.273											(3)1.714	(4)2.380	(5)2.939	(6)3.758	(7)4.368
																(3)2.164		
III		Na	Mg											Al	Si	P	S	Cl
	χ_i	(1)1.024	(2)1.234											(3)1.513	(4)1.887	(5)2.139	(6)2.659	(7)3.008
																(3)1.642	(4)1.973	(5)2.274
IV		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
	χ_i	(1)0.998	(2)1.160	(3)1.415	(4)1.730	(5)2.030	(6)2.475	(7)2.651	(3L)1.651	(3L)1.693	(4)2.037	(2)1.372	(2)1.336	(3)1.579	(4)1.854	(5)2.159	(6)2.448	(7)2.744
					(3)1.499	(4)1.795	(3)1.587	(4)1.912	(3H)1.556	(3H)1.621	(3L)1.695	(1)1.163			(2)1.314	(3)1.589	(4)1.869	(5)2.107
					(2)1.225	(3)1.545	(2L)1.322	(2L)1.343	(2L)1.390	(2L)1.377	(3H)1.650							
						(2)1.267	(2H)1.287	(2H)1.263	(2H)1.292	(2H)1.321	(2)1.367							
V		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
	χ_i	(1)0.998	(2)1.139	(3)1.340	(4)1.610	(5)1.862	(6)2.101	(7)2.384	(5)2.099	(5)2.167	(4)1.876	(2)1.333	(2)1.276	(3)1.480	(4)1.706	(5)1.971	(6)2.180	(7)2.417
						(4)1.690	(5)2.006	(5)2.002	(4)1.848	(4)1.863	(3)1.562	(1)1.097			(2)1.181	(3)1.476	(4)1.467	(5)1.587
						(3)1.501	(4)1.808	(4)1.773	(3)1.576	(3)1.622	(2)1.346							
VI		Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
	χ_i	(1)0.998	(2)1.126	(3)1.327	(4)1.706	(5)1.925	(6)2.175	(7)2.507	(7)2.573	(5)2.183	(5)2.159	(5)2.195	(2)1.326	(3)1.524	(4)1.746	(5)1.895	(6)2.168	(7)2.423
						(4)1.735	(5)1.991	(6)2.317	(6)2.362	(4)1.881	(4)1.895	(3)1.550	(1)1.165	(1)1.050	(2)1.225	(3)1.399	(4)1.575	
						(3)1.536	(4)1.784	(4)1.853	(4)1.888	(3)1.649	(2)1.432	(1)1.113						
VII		Fr	Ra	Ac	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
	χ_i	(1)1.012	(2)1.151	(3)1.363	(4)1.608	(4)1.646	(3)1.382	(3)1.391	(3)1.410	(3)1.433	(3)1.386	(4)1.733	(3)1.426	(3)1.433	(3)1.438	(3)1.455	(3)1.479	(3)1.431
					(3)1.348	(3)1.374				(2)1.181		(3)1.410	(2)1.213			(2)1.231	(2)1.237	

*The numbers in parentheses are oxidation states, "L" means low-spin and "H" means high-spin.

bond after the charge has been exchanged between them, which directly led to a new definition of ionic character in terms of charge transferred between the bond-forming orbitals[35]. In 1987, under the framework of density functional theory, Ghosh proposed another definition for bond EN. He divided a chemical bond into three regions: the two atomic sites and one bond region. Because the bond EN is higher than the average EN of two bonded atoms before bond formation, electrons flow from atom sites to the bond region, which explains the bonding process of homonuclear diatomic molecules[36]. Yang et al. established the atom-bond EN equalization method on the basis of density functional theory and EN equalization principle, which is applied to the calculation of charge distribution in large organic and biological molecules[37].

Considering the chemical environment of atoms in materials, we defined an EN scale of elements in covalent crystals, and proposed a new expression of bond EN, which was successfully used to identify the hardness of materials. In covalent crystals, the EN of element *w* is expressed as the electrostatic potential at the covalent boundary of the element caused by its nuclear charge shielded by the inner electrons, i.e., covalent potential, which is expressed as $\varphi_w = n_w/R_w$, where n_w is the number of bonding electrons, and R_w is the crystalline covalent radius[38]. We assign an EN of 2.55 (according to the Pauling scale in Table 1) to tetrahedral carbon in diamond, the most typical covalently bonded element, and thus EN values of elements in covalent crystals can be expressed by the following equation

$$\chi_w = 2.55/5.20\varphi_w = 0.49 n_w / R_w , \tag{3}$$

where 5.20 is the covalent potential of tetrahedral carbon. For a covalent bond a—b with coordination numbers CN_a and CN_b of atoms a and b, the bond is composed of $(1/CN_a)$ a atom and $(1/CN_b)$ b atom. Based on the idea of EN equalization, the bond EN can be defined as the average EN of two atoms distributed on the a—b bond[39]

$$X_{ab} = \sqrt{\frac{\chi_a}{CN_a}\frac{\chi_b}{CN_b}} , \tag{4}$$

where χ_a and χ_b are the EN of atoms a and b. EN represents the ability of an atom to attract or hold electrons, therefore bond EN X_{ab} represents the electron-holding power of this covalent bond, which reflects the strength of the covalent bond. If two bonded atoms a and b have different EN, the electron pair will be displaced from the bond center to the atom with a higher EN. The relatively weak part of the electron-holding energy will result in the decrease of the entire electron-holding energy of the bond. A correction factor $\exp(-\delta f_i)$ is thus introduced to express such an effect, where $f_i = 0.25|\chi_a - \chi_b| / \sqrt{\chi_a \chi_b}$. Combined with the density of chemical bonds $N_v = N/V$, where N is the number of covalent bonds per unit cell, and V is the volume of unit cell, we plot the experimental hardness data against $N_v X_{ab} \exp(-\delta f_i)$ for some typical covalent crystals. The microscopic model for identifying the hardness of materials is determined through a linear regression

$$H = 423.8 \frac{N}{V} \sqrt{\frac{\chi_a}{CN_a} \frac{\chi_b}{CN_b}} e^{-2.7 f_i} - 3.4, \qquad (5)$$

where 423.8 and –3.4 are fitting constants, in units of GPa·Å^4 and GPa. According to eq. (5), the larger EN product and the smaller EN difference are the necessary conditions for two atoms to form superhard materials. By using this model, the hardness of various materials can be satisfactorily predicted solely in terms of the EN of constituent atoms and crystal structure data. The elemental combinations that may form superhard materials are selected, which provides a useful guide for the design of new superhard materials. Bond EN is a bridge linking the EN of elements and the properties of materials, which directly establishes the quantitative relationship between the macroscopic properties and the microscopic structure of materials. Table 3 gives the recommended values of bond EN.

Table 3 Recommended values of bond electronegativity

Bond	X_{ab}	Bond	X_{ab}
C—C	0.637	In—N	0.473
S—Si	0.419	In—P	0.377
Ge—Ge	0.402	In—As	0.364
Sn—Sn	0.350	In—Sb	0.339
Si—C	0.516	Zn—S	0.364
B—N	0.605	Zn—Se	0.347
B—P	0.483	Zn—Te	0.323
B—As	0.466	C—N	0.878
Al—N	0.505	C—P	0.688
Al—P	0.403	Si—N	0.712
Al—As	0.389	Ti—C	0.310
Al—Sb	0.363	W—C	0.297
Ga—N	0.505	Be—O	0.507
Ga—P	0.403	Al—O	0.458
Ga—As	0.389	Sn—O	0.418
Ga—Sb	0.363	Mg—O	0.263

The study of the EN scale appears to have only limited theoretical or practical significance. The parameter of EN should be employed to study the nature of chemical bonds, establish the structure-property relationship, and guide materials design and synthesis. For example, Jansen et al. successfully synthesized perovskite-based inorganic yellow-red pigments through band gap tuning by adjusting the O/N ratio according to the EN of constituent elements[40]. Asahi et al. synthesized a photocatalyst with high reactivity under visible light by doping nitrogen into TiO_2 to reduce the band gap[41]. Their work provides a useful foundation for the application of EN.

4 Conclusions and prospects

The most important application of EN is that when combined with other atomic parameters, it is used to simplify complicated molecular phenomena and the properties of materials for some quantitative correlations. The EN values of constituent atoms determine the nature of chemical bonds, and further determine various physical and chemical properties of materials such as crystal structure, electron structure, non-linear optical polarizability, ultraviolet reflection coefficient and valence band photoemission. With the development of new materials, the concept of EN will have an important role in materials science. The construction of the structure-property relationship based on EN to predict the properties of materials and further design new materials is a major trend in the development of EN.

1 Pauling L. The Nature of the Chemical Bond. 3rd ed. New York: Cornell University Press, 1960

2 Wahl U, Rita E, Correia J G, et al. Direct evidence for As as a Zn-site impurity in ZnO. Phys Rev Lett, 2005, 95(21): 215503[doi]

3 Zhang L, Wang E, Xue Q, et al. Generalized electron counting in determination of metal-induced reconstruction of compound semiconductor surfaces. Phys Rev Lett, 2006, 97(12): 126103[doi]

4 Asokamani R, Manjula R. Correlation between electronegativity and superconductivity. Phys Rev B, 1989, 39(7): 4217—4221[doi]

5 Hur S G, Kim T W, Hwang S, et al. Synthesis of new visible light active photocatalysts of $Ba(In_{1/3}Pb_{1/3}M'_{1/3})O_3$ (M' = Nb, Ta): A band gap engineering strategy based on electronegativity of a metal component. J Phys Chem B 2005, 109(31): 15001—15007[doi]

6 Jiang J S, Du H L, Zhang W Y. Electronegativity, atomic pseudoradii and rare earth permanent magnet materials. J Chin Rare Earth Soc, 2003, 21(3): 287—290

7 Lebouteiller A, Courtine P J. Improvement of a bulk optical basicity table for oxidic systems. Solid State Chem, 1998, 137(1): 94—103[doi]

8 Mulliken R S. A new electroaffinity scale: together with data on valence states and on valence ionization potentials and electron affinities. J Chem Phys, 1934, 2(11): 782—793[doi]

9 Pauling L. The origin and nature of the electronegativity scale. J Chem Educ, 1988, 65(4): 375

10 Allred A L, Rochow E G. A scale of electronegativity based on electrostatic force. J Inorg Nucl Chem, 1958, 5(4): 264—268[doi]

11 Sanderson R T. An interpretation of bond lengths and a classification of bonds. Science, 1951, 114(2973): 670—672[doi]

12 Allen L C. Electronegativity is the average one-electron energy of the valence-shell electrons in ground-state free atoms. J Am Chem Soc, 1989, 111(25): 9003—9014[doi]

13 Phillips J C. Dielectric definition of electronegativity. Phys Rev Lett, 1968, 20(11): 550—553[doi]

14 Chen N Y, Chang H K. On the relationship between electronegativity and some parameters of atomic structure. Acta Chimica Sinica, 1975, 33(2): 101—112

15 Yuan H J. Studies on electronegativity. I. The electronegativity of atoms. Acta Chimica Sinica, 1964, 30(3): 341—347

16 Luo Y R, Benson S W. The covalent potential: a simple and useful measure of the valence-state electronegativity for correlating molecular energetics. Acc Chem Res, 1992, 25(8): 375—381[doi]

17 Iczkowski R P, Margrave J L. Electronegativity. J Am Chem Soc, 1961, 83(17): 3547[doi]

18 Parr R G, Donnelly R A, Levy M, et al. Electronegativity: The density functional viewpoint. J Chem Phys, 1978, 68(8): 3801—3807[doi]

19 Politzer P, Weinstein H. Some relations between electronic distribution and electronegativity. J Chem Phys, 1979, 71(11): 4218—4220[doi]

20 Sproul G. Electronegativity and bond type. 2. Evaluation of electronegativity scales. J Phys Chem, 1994, 98 (27): 6699—6703[doi]

21 Pearson R G. Electronegativity scales. Acc Chem Res, 1990, 23(1): 1—2[doi]

22 Allred A L, Rochow E G. Electronegativity values from thermochemical data. J Inorg Nucl Chem, 1961, 17 (3-4): 215—221[doi]

23 Frost R L, Erickson K L, Weier M L, et al. Use of infrared spectroscopy for the determination of electronegativity of rare earth elements. Appl Spectrosc, 2004, 58(7): 811—815[doi]

24 Leyssens T, Geerlings P, Peeters D. A group electronegativity equalization scheme including external potential effects. J Phys Chem A, 2006, 110(28): 8872—8879[doi]

25 Sanderson R T. Electronegativities in inorganic chemistry. J Chem Educ, 1954, 31(1): 2—7

26 Zhang Y H. Electronegativities of elements in valence states and their applications. Inorg Chem, 1982, 21(11): 3886—3893[doi]

27 Sanderson R T. Electronegativity and bonding of transitional elements. Inorg Chem, 1986, 25(19): 3518—3522[doi]

28 Li K, Xue D. Estimation of electronegativity values of elements in different valence states. J Phys Chem A, 2006, 110(39): 11332—11337[doi]

29 Asthagiri D, Pratt L R, Paulaitis M E, et al. Hydration structure and free energy of biomolecularly specific aqueous dications, including Zn^{2+} and first transition row metals. J Am Chem Soc, 2004, 126(4): 1285—1289[doi]

30 Su Q. Chemistry of Rare Earths. Zhengzhou: Henan Science and Technology Press, 1993

31 Li K, Xue D. A new set of electronegativity scale for trivalent lanthanides. Phys Stat Sol B, 2007, 244 (6): 1982—1987[doi]

32 Brown I D, Skowron A. Electronegativity and Lewis acid strength. J Am Chem Soc, 1990, 112(9): 3401—3403[doi]

33 Luo Y R, Benson S W. A new electronegativity scale. 12. Intrinsic Lewis acid strength for main-group elements. Inorg Chem, 1991, 30(7): 1677—1680[doi]

34 Tsuruta H, Yamaguchi K, Imamoto T, et al. Tandem mass spectrometric analysis of rare earth(III) complexes: evaluation of the relative strength of their Lewis acidity. Tetrahedron, 2003, 59(52): 10419—10438[doi]

35 Hinze J, Whitehead M A, Jaffe H H. Electronegativity. II. Bond and orbital electronegativities. J Am Chem Soc, 1963, 85(2): 148—154[doi]

36 Ghosh S K. Toward a semiempirical density functional theory of chemical binding. Theor Chim Acta, 1987, 72(5-6): 379—391[doi]

37 Cui B Q, Zhao D X, Yang Z Z. Prediction of reactive site in superoxide dismutase in terms of atom-bond electronegativity equalization method. Acta Chimica Sinica, 2007, 65(23): 2687—2692

38 Li K, Wang X, Xue D. Electronegativities of elements in covalent crystals. J Phys Chem A, 2008, 112(34): 7894—7897[doi]

39 Li K, Wang X, Zhang F, et al. Electronegativity identification of novel superhard materials. Phys Rev Lett, 2008, 100(23): 235504[doi]

40 Jansen M, Letschert H P. Inorganic yellow-red pigments without toxic metals. Nature, 2000, 404(6781): 980—982[doi]

41 Asahi R, Morikawa T, Ohwaki T, et al. Visible-light photocatalysis in nitrogen-doped titanium oxides. Science, 2001, 293(5528): 269—271[doi]