Supporting Information

Identification of biomolecule-based electronic materials from a first-principles study of aliphatic amino acids

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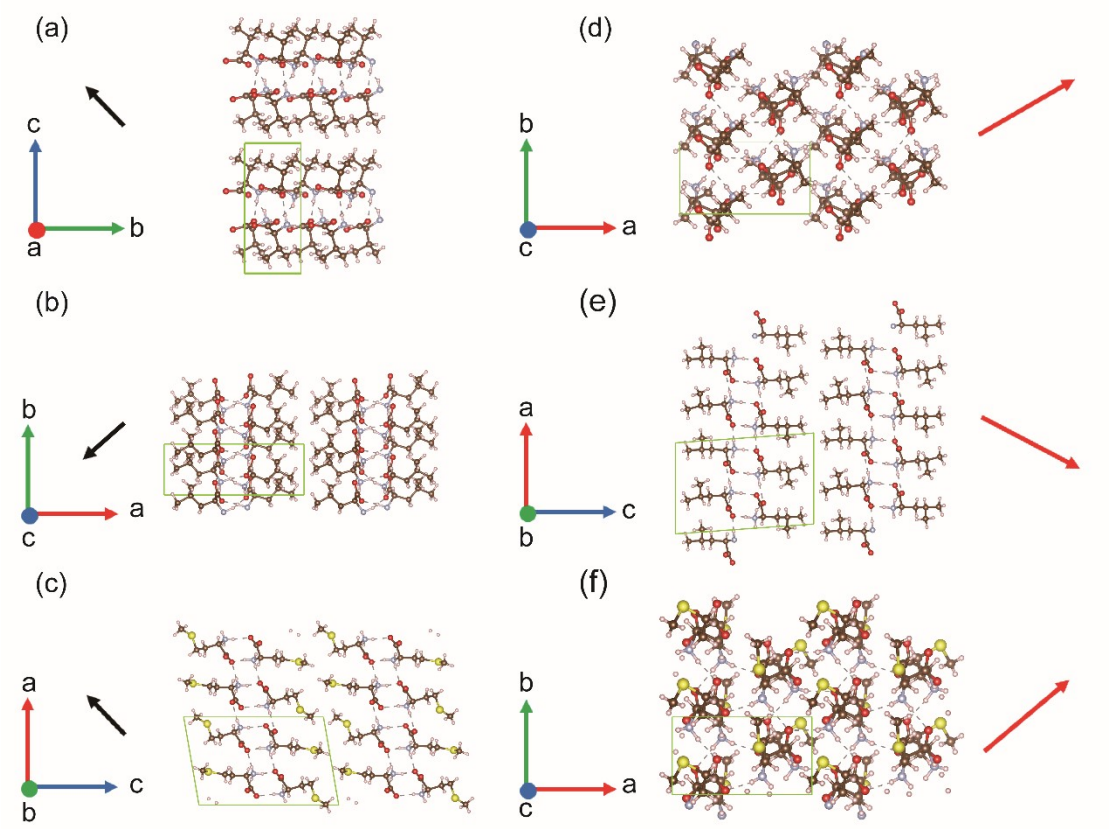

Fig. S1 Directions of the minimal (black arrow) and maximal (red arrow) Young's modulus value of L-Val, L-Leu, and L-Met. Projection of L-Val along (a) a-axis and (d) c-axis. Projection of L-Leu along (b) c-axis and (e) b-axis. Projection of L-Met along (c) b-axis and (f) c-axis.

Table S1 Calculated dielectric tensor $\boldsymbol{\varepsilon}_{ij}$ of L-Val, L-Leu, and L-Met

$$\boldsymbol{\varepsilon}_{ij\_L\text{-}Val} = \begin{bmatrix} 2.616 & 0 & 0.103 \\ 0 & 2.676 & 0 \\ 0.103 & 0 & 2.498 \end{bmatrix}$$

$$\boldsymbol{\varepsilon}_{ij\_L\text{-}Leu} = \begin{bmatrix} 2.325 & 0 & 0.083 \\ 0 & 2.409 & 0 \\ 0.083 & 0 & 2.298 \end{bmatrix}$$

$$\boldsymbol{\varepsilon}_{ij\_L\text{-}Met} = \begin{bmatrix} 2.754 & 0 & 0.234 \\ 0 & 2.730 & 0 \\ 0.234 & 0 & 3.291 \end{bmatrix}$$

Table S2 Calculated piezoelectric stress tensor $\boldsymbol{e}_{ij}$ of L-Val, L-Leu, and L-Met (C/m^2)

$$\boldsymbol{e}_{ij\_L\text{-}Val} = \begin{bmatrix} 0 & 0 & 0 & -0.044 & 0 & -0.004 \\ -0.123 & -0.253 & 0.024 & 0 & -0.029 & 0 \\ 0 & 0 & 0 & -0.009 & 0 & -0.029 \end{bmatrix}$$

$$\boldsymbol{e}_{ij\_L\text{-}Leu} = \begin{bmatrix} 0 & 0 & 0 & 0.500 & 0 & -0.639 \\ 0.107 & -0.214 & -0.109 & 0 & 0.165 & 0 \\ 0 & 0 & 0 & -0.279 & 0 & -0.279 \end{bmatrix}$$

$$\boldsymbol{e}_{ij\_L\text{-}Met} = \begin{bmatrix} 0 & 0 & 0 & -0.070 & 0 & 0.016 \\ 0.202 & 0.201 & 0.046 & 0 & 0.022 & 0 \\ 0 & 0 & 0 & -0.103 & 0 & 0.071 \end{bmatrix}$$

Table S3 Calculated piezoelectric strain tensor $\boldsymbol{d}_{ij}$ of L-Val (pm/V)

$$\boldsymbol{d}_{ij\_L\text{-}Val} = \begin{bmatrix} 0 & 0 & 0 & -9.486 & 0 & -1.985 \\ -0.180 & 7.26 & 3.931 & 0 & -4.580 & 0 \\ 0 & 0 & 0 & -3.030 & 0 & -2.400 \end{bmatrix}$$

$$\boldsymbol{d}_{ij\_L\text{-}Leu} = \begin{bmatrix} 0 & 0 & 0 & -56.280 & 0 & -3.050 \\ 10.124 & -15.11 & -1.860 & 0 & 41.953 & 0 \\ 0 & 0 & 0 & -23.200 & 0 & -44.060 \end{bmatrix}$$

$$\boldsymbol{d}_{ij\_L\text{-}Met} = \begin{bmatrix} 0 & 0 & 0 & -9.280 & 0 & -2.580 \\ 4.436 & 9.023 & -0.870 & 0 & 9.562 & 0 \\ 0 & 0 & 0 & -11.060 & 0 & -0.130 \end{bmatrix}$$

Table S4 Calculated piezoelectric voltage tensor $\boldsymbol{g}_{ij}$ of L-Val, L-Leu, and L-Met (V mN^{-1})

$$\boldsymbol{g}_{ij\_L\text{-}Val} = \begin{bmatrix} 0 & 0 & 0 & -0.412 & 0 & -0.086 \\ -0.008 & 0.316 & 0.171 & 0 & -0.199 & 0 \\ 0 & 0 & 0 & -0.132 & 0 & -0.104 \end{bmatrix}$$

$$\boldsymbol{g}_{ij\_L\text{-}Leu} = \begin{bmatrix} 0 & 0 & 0 & -2.706 & 0 & -0.147 \\ 0.006 & -0.727 & -0.089 & 0 & 2.017 & 0 \\ 0 & 0 & 0 & -1.116 & 0 & -2.119 \end{bmatrix}$$

$$\boldsymbol{g}_{ij\_L\text{-}Met} = \begin{bmatrix} 0 & 0 & 0 & -0.358 & 0 & -0.100 \\ 0.171 & 0.348 & -0.034 & 0 & 0.369 & 0 \\ 0 & 0 & 0 & -0.427 & 0 & -0.005 \end{bmatrix}$$

Table S5 Calculated elastic stiffness tensor $\boldsymbol{C}_{ij}$ of L-Val

$$\boldsymbol{C}_{ij\_L\text{-}Val} = \begin{bmatrix} 55.167 & 23.875 & 15.680 & 0 & 0.257 & 0 \\ 23.875 & 40.721 & 10.617 & 0 & -1.151 & 0 \\ 15.680 & 10.617 & 29.745 & 0 & 2.836 & 0 \\ 0 & 0 & 0 & 5.237 & 0 & -2.862 \\ 0.257 & -1.151 & 2.836 & 0 & 10.589 & 0 \\ 0 & 0 & 0 & -2.862 & 0 & 15.692 \end{bmatrix}$$

$$\boldsymbol{C}_{ij\_L\text{-}Leu} = \begin{bmatrix} 12.221 & 1.619 & 1.110 & 0 & -0.552 & 0 \\ 1.619 & 22.443 & 13.345 & 0 & -0.672 & 0 \\ 1.110 & 13.345 & 28.015 & 0 & -4.206 & 0 \\ 0 & 0 & 0 & 7.677 & 0 & 2.226 \\ -0.552 & -0.672 & -4.206 & 0 & 3.348 & 0 \\ 0 & 0 & 0 & 2.226 & 0 & 2.487 \end{bmatrix}$$

$$\boldsymbol{C}_{ij\_L\text{-}Met} = \begin{bmatrix} 27.725 & 7.531 & 7.542 & 0 & 1.842 & 0 \\ 7.531 & 20.854 & 2.544 & 0 & -1.920 & 0 \\ 7.542 & 2.544 & 23.537 & 0 & 1.049 & 0 \\ 0 & 0 & 0 & 9.389 & 0 & -6.624 \\ 1.842 & -1.920 & 1.049 & 0 & 3.353 & 0 \\ 0 & 0 & 0 & -6.624 & 0 & 17.612 \end{bmatrix}$$

Table S6 Calculated elastic compliance tensor $\boldsymbol{S}_{ij}$ of L-Val, L-Leu, and L-Met

$$\boldsymbol{S}_{ij\_L\text{-}Val} = \begin{bmatrix} 0.026 & -0.013 & -0.009 & 0 & 0.000 & 0 \\ -0.013 & 0.034 & -0.006 & 0 & 0.006 & 0 \\ -0.009 & -0.006 & 0.042 & 0 & -0.012 & 0 \\ 0 & 0 & 0 & 0.212 & 0 & 0.039 \\ 0.000 & 0.006 & -0.012 & 0 & 0.098 & 0 \\ 0 & 0 & 0 & 0.039 & 0 & 0.071 \end{bmatrix}$$

$$\boldsymbol{S}_{ij\_L\text{-}Leu} = \begin{bmatrix} 0.033 & -0.025 & 0.013 & 0 & 0.015 & 0 \\ -0.025 & 0.054 & 0.026 & 0 & 0.012 & 0 \\ 0.013 & 0.026 & -0.017 & 0 & 0.003 & 0 \\ 0 & 0 & 0 & -0.003 & 0 & 0.086 \\ 0.015 & 0.012 & 0.003 & 0 & 0.262 & 0 \\ 0 & 0 & 0 & 0.086 & 0 & 0.072 \end{bmatrix}$$

$$\boldsymbol{S}_{ij\_L\text{-}Met} = \begin{bmatrix} 0.046 & -0.018 & -0.011 & 0 & -0.032 & 0 \\ -0.018 & 0.059 & -0.002 & 0 & 0.045 & 0 \\ -0.011 & -0.002 & 0.047 & 0 & -0.010 & 0 \\ 0 & 0 & 0 & 0.145 & 0 & 0.055 \\ -0.032 & 0.045 & -0.010 & 0 & 0.345 & 0 \\ 0 & 0 & 0 & 0.055 & 0 & 0.077 \end{bmatrix}$$

Table S7 Calculated elastic constants of L-Val

Scheme	Voigt	Reuss	Hill
Bulk Modulus *B* (GPa)	25.109	21.850	23.479
Shear Modulus *G* (GPa)	11.334	9.019	10.177
Young's Modulus *E* (GPa)	29.556	23.785	26.676
P-wave Modulus (GPa)	40.221	33.876	37.048
Poisson's Ratio *v*	0.304	0.319	0.311
Bulk/Shear Ratio	2.215	2.423	2.307

Table S8 Calculated elastic constants of L-Leu

Scheme	Voigt	Reuss	Hill
Bulk Modulus *B* (GPa)	10.536	7.614	9.075
Shear Modulus *G* (GPa)	5.809	3.466	4.638
Young's Modulus *E* (GPa)	14.722	9.029	11.888
P-wave Modulus (GPa)	18.282	12.236	15.259
Poisson's Ratio v	0.267	0.302	0.282
Bulk/Shear Ratio	1.814	2.197	1.957

Table S9 Calculated elastic constants of L-Met

Scheme	Voigt	Reuss	Hill
Bulk Modulus *B* (GPa)	11.928	11.404	11.666
Shear Modulus *G* (GPa)	9.704	6.153	7.928
Young's Modulus *E* (GPa)	22.901	15.645	19.392
P-wave Modulus (GPa)	24.866	19.607	22.237
Poisson's Ratio *v*	0.180	0.271	0.223
Bulk/Shear Ratio	1.229	1.853	1.471

Table S10 Analysis of the unit cell parameters of three amino acids crystals calculated with and without dispersion corrections.

		a(Å)	b(Å)	c(Å)	β(°)	E_0(eV)
L-Val	DFT	9.538	5.176	11.625	90.704	-436.651
	DFT-D3	9.453	5.070	11.204	90.138	-441.271
	error	0.085	0.106	0.421	0.566	4.62
	error ratio(%)	0.899	2.091	3.758	0.628	1.047
L-Leu	DFT	9.606	5.324	14.666	94.060	-507.663
	DFT-D3	9.357	5.146	13.978	94.007	-508.406
	error	0.249	0.178	0.688	0.053	0.743
	error ratio(%)	2.661	3.459	4.922	0.056	0.146
L-Met	DFT	9.333	5.066	14.325	96.076	-387.519
	DFT-D3	9.259	4.960	14.086	96.243	-392.447
	error	0.074	0.106	0.239	-0.167	4.928
	error ratio(%)	0.799	2.137	1.700	0.174	1.256

Table S11 Analysis of the unit cell parameters of three amino acids crystals calculated with conventional DFT and MP2 method.

		a(Å)	b(Å)	c(Å)	β(°)
L-Val	DFT	9.538	5.176	11.625	90.704
	MP2	9.453	5.070	11.204	90.138
	error	0.085	0.106	0.421	0.566
	error ratio(%)	0.899	2.091	3.758	0.627
L-Leu	DFT	9.606	5.324	14.666	94.060
	MP2	9.357	5.146	13.978	94.007
	error	0.249	0.178	0.688	0.053
	error ratio(%)	2.661	3.459	4.922	0.056
L-Met	DFT	9.333	5.066	14.325	96.076

	MP2	9.259	4.960	14.086	96.243
	error	0.074	0.106	0.239	0.167
	error ratio(%)	0.799	2.137	1.700	0.174