## Electronic Supplementary Information

# Computational predictions turning the isomers of alanine to generate distinct morphs of free flowing salt crystals

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## Complete Gaussian reference

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision B01, Gaussian, Inc., Wallingford, CT, 2010.

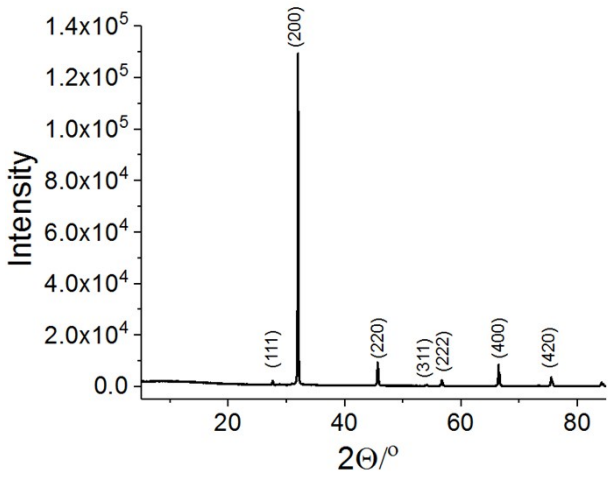



**Figure S1** The powder- XRD patterns of the homogeneous NaCl crystals obtained from pure saturated NaCl solution.

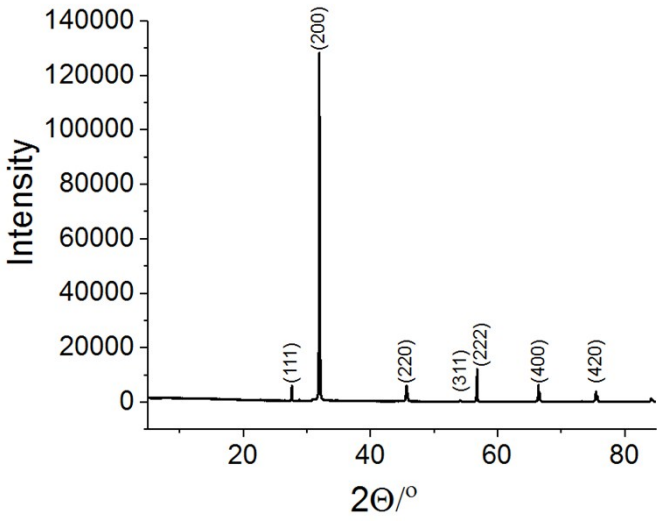



**Figure S2** The powder- XRD patterns of the homogeneous NaCl crystals obtained from 30% (w/v) α-alanine contaminated saturated NaCl solution.

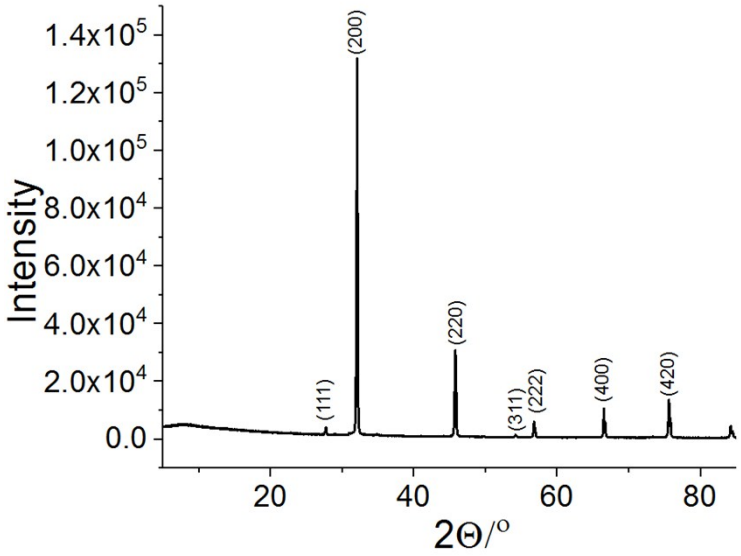



**Figure S3** The powder- XRD patterns of the homogeneous NaCl crystals obtained from 30% (w/v) β-alanine contaminated saturated NaCl solution.

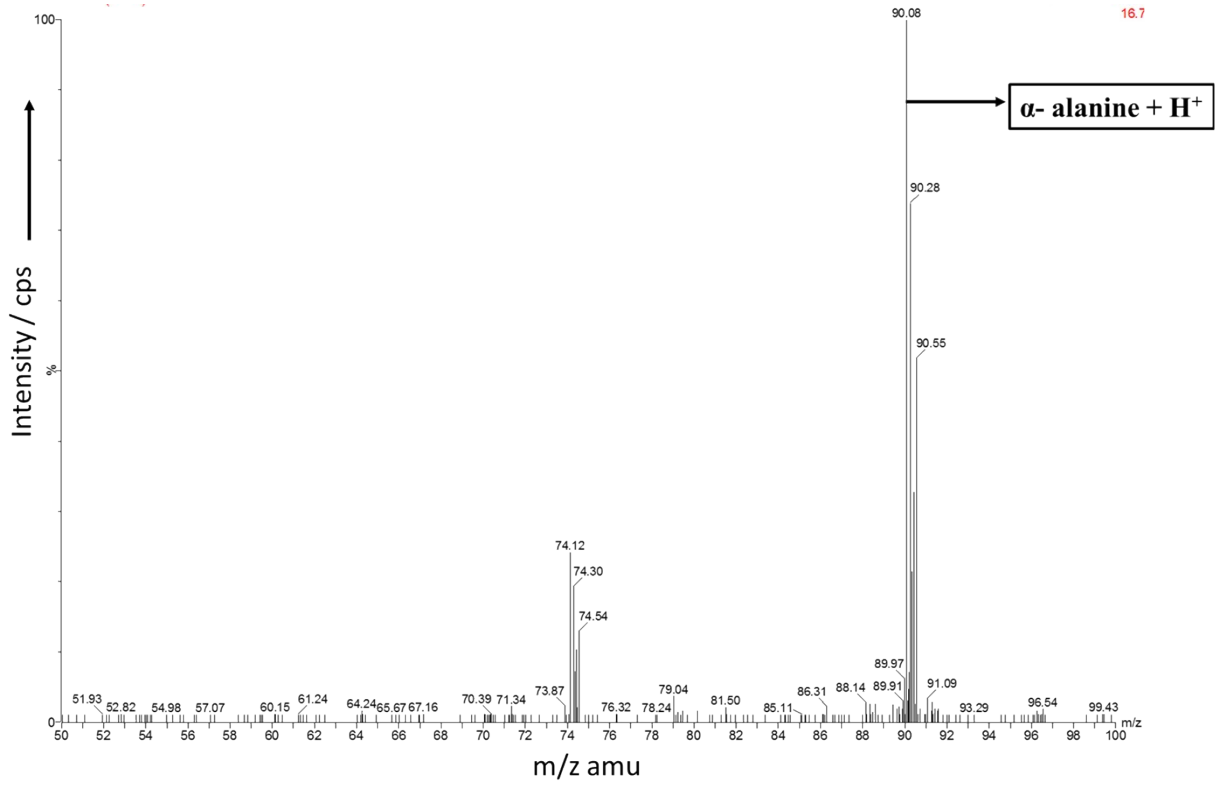



**Figure S4** ESI-MS spectrum of α-alanine.

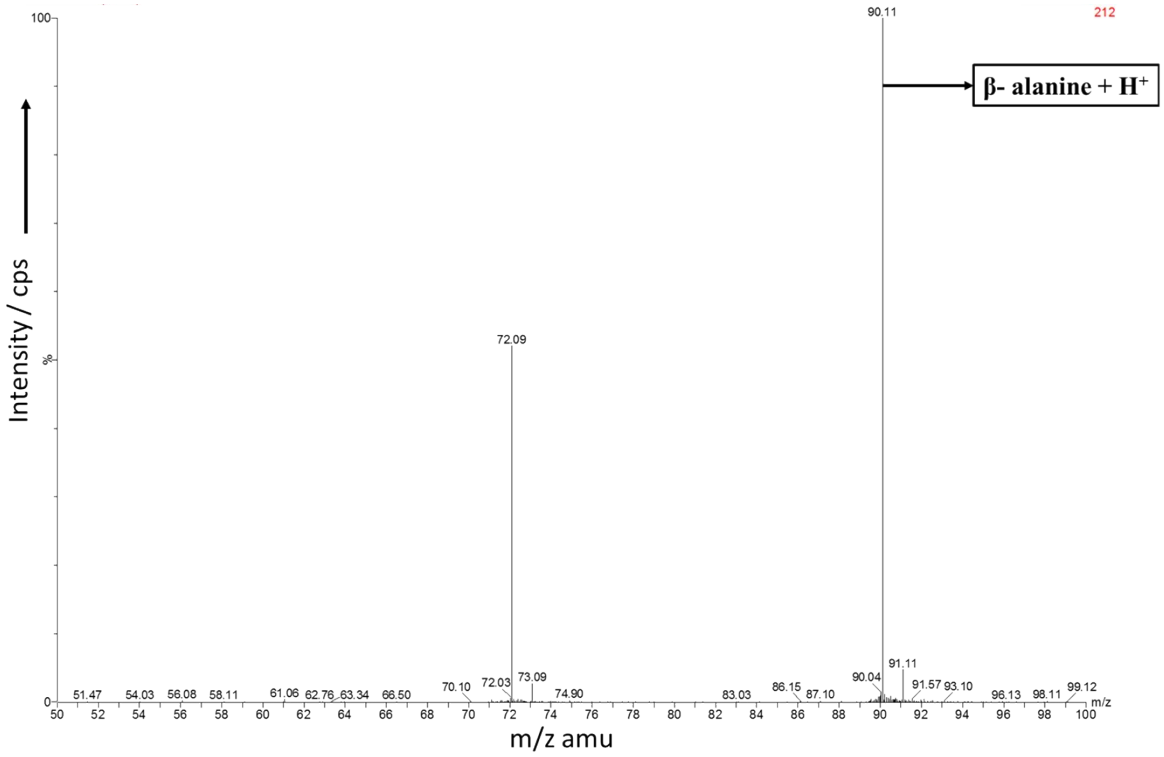
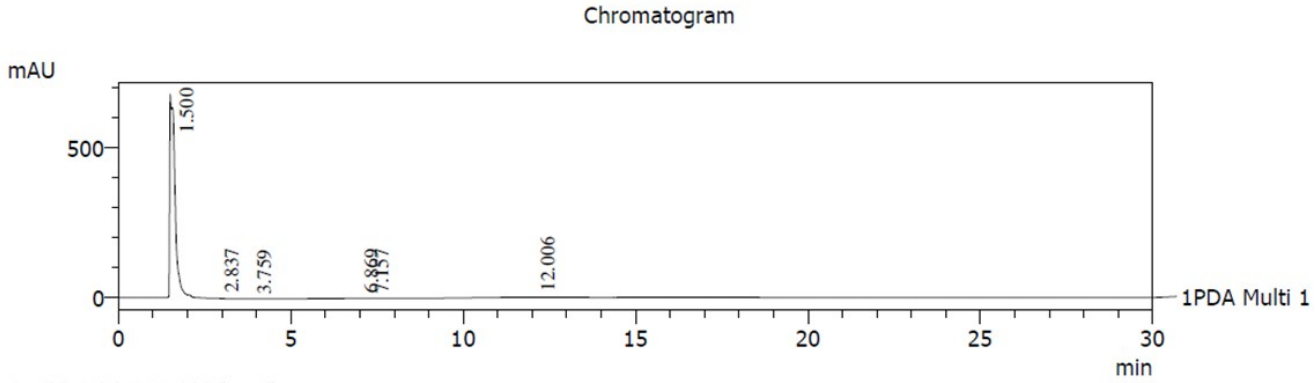



**Figure S5** ESI-MS spectrum of β-alanine.



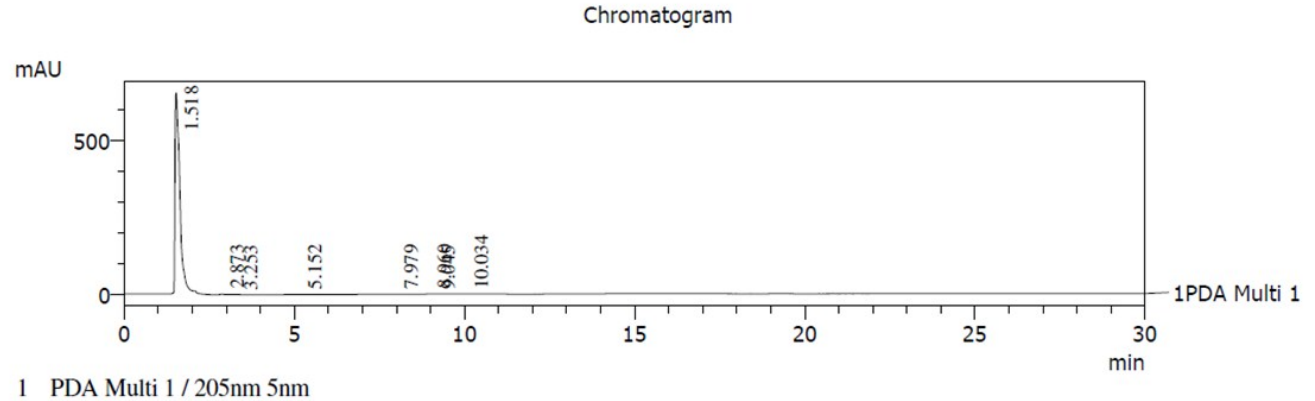

1 PDA Multi 1 / 205nm 5nm

PeakTable

PDA Ch1 205nm 5nm

| Peak# | Ret. Time | Area | Area % |
|---|---|---|---|
| 1 | 1.500 | 7354194 | 99.636 |
| 2 | 2.837 | 7379 | 0.100 |
| 3 | 3.759 | 1509 | 0.020 |
| 4 | 6.869 | 15467 | 0.210 |
| 5 | 7.157 | 1035 | 0.014 |
| 6 | 12.006 | 1486 | 0.020 |
| Total | | 7381071 | 100.000 |

**Figure S6** HPLC (High-performance liquid chromatography) Curve of α-alanine.




1 PDA Multi 1 / 205nm 5nm

PeakTable

PDA Ch1 205nm 5nm

| Peak# | Ret. Time | Area | Area % |
|---|---|---|---|
| 1 | 1.518 | 6621177 | 98.833 |
| 2 | 2.873 | 24624 | 0.368 |
| 3 | 3.253 | 37408 | 0.558 |
| 4 | 5.152 | 10649 | 0.159 |
| 5 | 7.979 | 1486 | 0.022 |
| 6 | 8.960 | 1052 | 0.016 |
| 7 | 9.045 | 1012 | 0.015 |
| 8 | 10.034 | 1944 | 0.029 |
| Total | | 6699351 | 100.000 |

**Figure S7** HPLC (High-performance liquid chromatography) Curve of β-alanine.

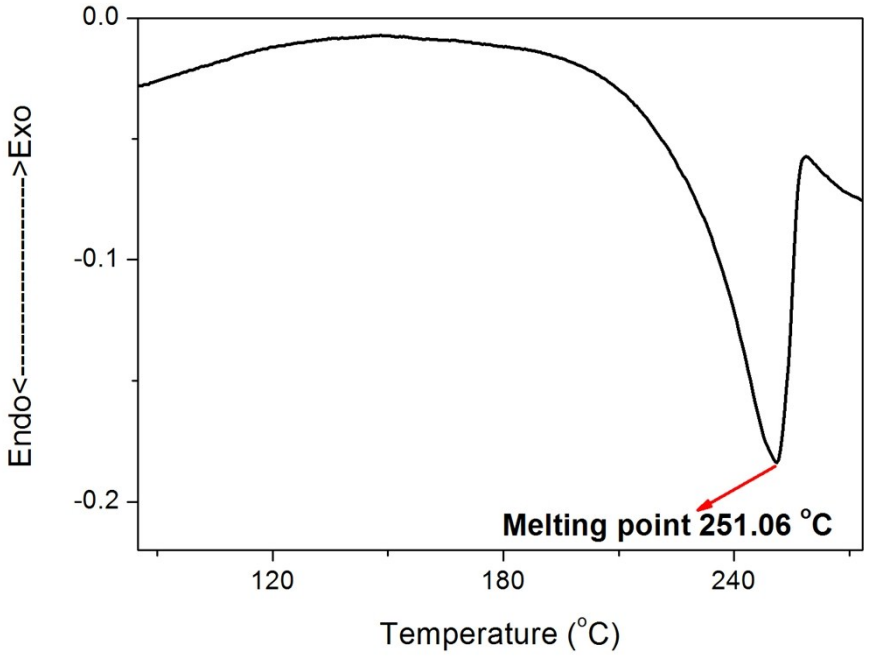



**Figure S8** DSC Curve of α-alanine showing the melting point measurements.

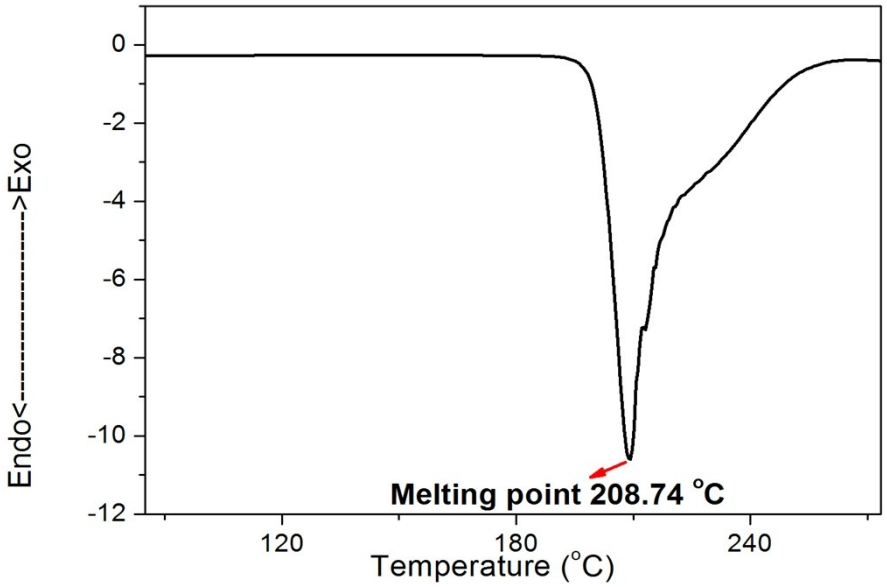


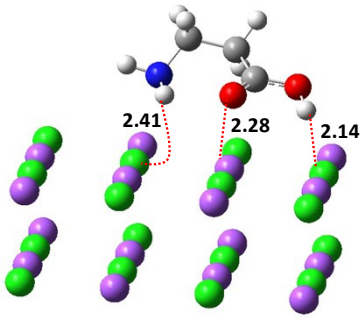

**Figure S9** DSC Curve of β-alanine showing the melting point measurements.

**Table TS1.** CHN analysis of α-alanine.

| | C | H | N |
|---|---|---|---|
| Chem Biodraw analysis data for α-alanine | 40.44% | 7.92% | 15.72% |
| Experimental analysis data for α-alanine | 40.45% | 7.90% | 15.66% |

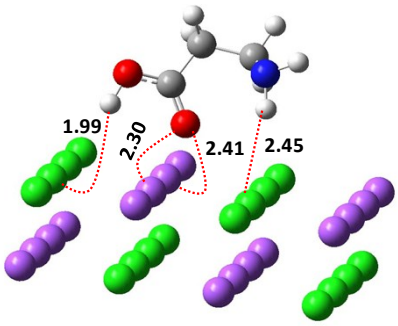
**Table TS2.** CHN analysis of β-alanine.

| | C | H | N |
|---|---|---|---|
| Chem Biodraw analysis data for β-alanine | 40.44% | 7.92% | 15.72% |
| Experimental analysis data for β-alanine | 40.46% | 7.79% | 15.68% |



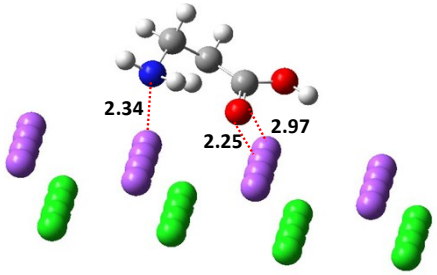

β-alanine-100

(-24.3 kcal/mol)




β-alanine-110

(-25.4 kcal/mol)




β-alanine-111

(-20.0 kcal/mol)

**Figure S10** BSSE corrected energies (kcal/mol) Calculated at the M06-2X/6-31+G(d) level for β-alanine with {100}, {110}, and {111} Surfaces of NaCl derived from slab model. (The interaction energies are given in bracket).