SUPPLEMENTARY INFORMATION

Becquerelite mineral phase: crystal structure and thermodynamic and mechanic stability by using periodic DFT

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Table S.1. Calculated isobaric heat capacity function, \( C_P \), of becquerelite. Temperature and heat capacity values are given in \( K \) and \( J \cdot K^{-1} \cdot \text{mol}^{-1} \) units, respectively.

| \( T \) | \( C_P \) | \( T \) | \( C_P \) | \( T \) | \( C_P \) |
|-------|--------|-------|--------|-------|--------|
| 10    | 1.59646 | 350   | 158.73070 | 690   | 193.50098 |
| 20    | 6.74505 | 360   | 160.46961 | 700   | 194.10347 |
| 30    | 13.95060 | 370   | 162.13674 | 710   | 194.69408 |
| 40    | 22.20754 | 380   | 163.73601 | 720   | 195.27332 |
| 50    | 30.92287 | 390   | 165.27110 | 730   | 195.84167 |
| 60    | 39.65372 | 400   | 166.74548 | 740   | 196.39958 |
| 70    | 48.11604 | 410   | 168.16244 | 750   | 196.94747 |
| 80    | 56.15642 | 420   | 169.52506 | 760   | 197.48575 |
| 90    | 63.70929 | 430   | 170.83629 | 770   | 198.01466 |
| 100   | 70.76223 | 440   | 172.09887 | 780   | 198.54974 |
| 110   | 77.33249 | 450   | 173.31543 | 790   | 199.04646 |
| 120   | 83.45203 | 460   | 174.48844 | 800   | 199.54974 |
| 130   | 89.15862 | 470   | 175.62023 | 810   | 200.04503 |
| 140   | 94.49062 | 480   | 176.71301 | 820   | 200.53261 |
| 150   | 99.48419 | 490   | 177.76886 | 830   | 201.01272 |
| 160   | 104.17209 | 500   | 178.79777 | 840   | 201.48559 |
| 170   | 108.58321 | 510   | 179.77759 | 850   | 201.95146 |
| 180   | 112.74272 | 520   | 180.73409 | 860   | 202.41051 |
| 190   | 116.67242 | 530   | 181.66093 | 870   | 202.86296 |
| 200   | 120.39118 | 540   | 182.55967 | 880   | 203.30897 |
| 210   | 123.91541 | 550   | 183.43181 | 890   | 203.74873 |
| 220   | 127.25944 | 560   | 184.27873 | 900   | 204.18238 |
| 230   | 130.43596 | 570   | 185.10177 | 910   | 204.61010 |
| 240   | 133.45622 | 580   | 185.90215 | 920   | 205.03201 |
| 250   | 136.33036 | 590   | 186.68104 | 930   | 205.44825 |
| 260   | 139.06756 | 600   | 187.43955 | 940   | 205.85896 |
| 270   | 141.67618 | 610   | 188.17872 | 950   | 206.26425 |
| 280   | 144.16391 | 620   | 188.89952 | 960   | 206.64424 |
| 290   | 146.53785 | 630   | 189.60286 | 970   | 207.05903 |
| 300   | 148.80458 | 640   | 190.28960 | 980   | 207.44873 |
| 310   | 150.97022 | 650   | 190.96055 | 990   | 207.83344 |
| 320   | 153.04047 | 660   | 191.61648 | 1000  | 208.21325 |
| 330   | 155.02068 | 670   | 192.25809 |  -    |  -        |
| 340   | 156.91586 | 680   | 192.88604 |  -    |  -        |
Table S.2. Calculated entropy function, $S$, of becquerelite. Temperature and entropy values are given in $K$ and $J\cdot K^{-1} \cdot mol^{-1}$ units, respectively.

| $T$  | $S$   | $T$  | $S$   | $T$  | $S$   |
|------|-------|------|-------|------|-------|
| 10   | 0.67942 | 350  | 196.97227 | 690  | 317.31869 |
| 20   | 3.20211 | 360  | 201.46840 | 700  | 320.10725 |
| 30   | 7.25114 | 370  | 205.88796 | 710  | 322.86477 |
| 40   | 12.37826 | 380  | 210.23328 | 720  | 325.59187 |
| 50   | 18.26548 | 390  | 214.50637 | 730  | 328.28924 |
| 60   | 24.67746 | 400  | 218.70933 | 740  | 330.95761 |
| 70   | 31.43067 | 410  | 222.84424 | 750  | 333.59755 |
| 80   | 38.38558 | 420  | 226.91301 | 760  | 336.20974 |
| 90   | 45.44057 | 430  | 230.91754 | 770  | 338.79471 |
| 100  | 52.52259 | 440  | 234.85955 | 780  | 341.35314 |
| 110  | 59.57859 | 450  | 238.74080 | 790  | 343.88557 |
| 120  | 66.57320 | 460  | 242.56298 | 800  | 346.39249 |
| 130  | 73.48069 | 470  | 246.32773 | 810  | 348.87447 |
| 140  | 80.28556 | 480  | 250.03671 | 820  | 351.33206 |
| 150  | 86.97670 | 490  | 253.69127 | 830  | 353.76569 |
| 160  | 93.54856 | 500  | 257.29301 | 840  | 356.17588 |
| 170  | 99.99759 | 510  | 260.84336 | 850  | 358.56309 |
| 180  | 106.32304 | 520  | 264.34359 | 860  | 360.92782 |
| 190  | 112.52496 | 530  | 267.79511 | 870  | 363.27046 |
| 200  | 118.60479 | 540  | 271.19912 | 880  | 365.59150 |
| 210  | 124.56486 | 550  | 274.55697 | 890  | 367.89129 |
| 220  | 130.40723 | 560  | 277.86978 | 900  | 370.17026 |
| 230  | 136.13468 | 570  | 281.13871 | 910  | 372.42878 |
| 240  | 141.75035 | 580  | 284.36493 | 920  | 374.66731 |
| 250  | 147.25704 | 590  | 287.54952 | 930  | 376.86814 |
| 260  | 152.65788 | 600  | 290.69348 | 940  | 379.08564 |
| 270  | 157.95557 | 610  | 293.79783 | 950  | 381.26622 |
| 280  | 163.15339 | 620  | 296.86357 | 960  | 383.42818 |
| 290  | 168.25392 | 630  | 299.89166 | 970  | 385.57183 |
| 300  | 173.26031 | 640  | 302.88303 | 980  | 387.69754 |
| 310  | 178.17520 | 650  | 305.83852 | 990  | 389.80556 |
| 320  | 183.00126 | 660  | 308.75896 | 1000 | 391.89627 |
| 330  | 187.74108 | 670  | 311.64534 | -    | -        |
| 340  | 192.39731 | 680  | 314.49831 | -    | -        |
Table S.3. Calculated enthalpy function, $\Delta H$ ($\Delta H = H_T - H_{298}$), of becquerelite. Temperature and enthalpy values are given in $K$ and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

| T  | $H_T - H_{298}$ | T  | $H_T - H_{298}$ | T  | $H_T - H_{298}$ |
|----|-----------------|----|-----------------|----|-----------------|
| 10 | -2629.36792     | 350| 22.77841        | 690| 99.87522        |
| 20 | -1312.71807     | 360| 26.57909        | 700| 101.21705       |
| 30 | -871.73489      | 370| 30.22050        | 710| 102.52951       |
| 40 | -649.29751      | 380| 33.71311        | 720| 103.81361       |
| 50 | -514.12810      | 390| 37.06691        | 730| 105.07035       |
| 60 | -422.55649      | 400| 40.29052        | 740| 106.30078       |
| 70 | -355.91743      | 410| 43.39217        | 750| 107.50575       |
| 80 | -304.90595      | 420| 46.37925        | 760| 108.68620       |
| 90 | -264.36377      | 430| 49.25843        | 770| 109.84288       |
| 100| -231.19955      | 440| 52.03597        | 780| 110.97661       |
| 110| -203.44644      | 450| 54.71768        | 790| 112.08819       |
| 120| -179.79019      | 460| 57.30875        | 800| 113.17832       |
| 130| -159.31877      | 470| 59.81402        | 810| 114.24774       |
| 140| -141.37785      | 480| 62.23811        | 820| 115.29700       |
| 150| -125.48493      | 490| 64.58516        | 830| 116.32685       |
| 160| -111.27635      | 500| 66.85907        | 840| 117.33782       |
| 170| -98.47191       | 510| 69.06351        | 850| 118.33053       |
| 180| -86.85232       | 520| 71.20188        | 860| 119.30558       |
| 190| -76.24298       | 530| 73.27731        | 870| 120.26340       |
| 200| -66.50322       | 540| 75.29284        | 880| 121.20456       |
| 210| -57.51894       | 550| 77.25109        | 890| 122.12958       |
| 220| -49.19518       | 560| 79.15476        | 900| 123.03887       |
| 230| -41.45364       | 570| 81.00631        | 910| 123.93291       |
| 240| -34.22809       | 580| 82.80795        | 920| 124.81214       |
| 250| -27.46286       | 590| 84.56200        | 930| 125.67696       |
| 260| -21.10995       | 600| 86.27031        | 940| 126.52779       |
| 270| -15.12876       | 610| 87.93488        | 950| 127.36497       |
| 280| -9.48392        | 620| 89.55755        | 960| 128.18891       |
| 290| -4.14450        | 630| 91.14000        | 970| 129.00000       |
| 300| 0.91641         | 640| 92.68393        | 980| 129.79851       |
| 310| 5.72214         | 650| 94.19068        | 990| 130.58479       |
| 320| 10.29372        | 660| 95.66189        | 1000| 131.35917      |
| 330| 14.64963        | 670| 97.09883        | -  | -               |
| 340| 18.80630        | 680| 98.50292        | -  | -               |
### Table S.4. Calculated free-energy function, $\Delta G (\Delta G = G_T - H_{298})$, of becquerelite. Temperature and free-energy values are given in K and $J\cdot K^{-1}\cdot mol^{-1}$ units, respectively.

| T   | $G_T - H_{298}$ | T   | $G_T - H_{298}$ | T   | $G_T - H_{298}$ |
|-----|-----------------|-----|-----------------|-----|-----------------|
| 10  | -2630.04781     | 350 | -174.19387      | 690 | -217.44347      |
| 20  | -1315.92018     | 360 | -174.88921      | 700 | -218.89021      |
| 30  | -878.98603      | 370 | -175.66746      | 710 | -220.33526      |
| 40  | -661.67477      | 380 | -176.52007      | 720 | -221.77826      |
| 50  | -532.39358      | 390 | -177.43946      | 730 | -223.21884      |
| 60  | -447.23395      | 400 | -178.41881      | 740 | -224.65677      |
| 70  | -387.34810      | 410 | -179.45207      | 750 | -226.09174      |
| 80  | -343.29153      | 420 | -180.53377      | 760 | -227.52354      |
| 90  | -309.80434      | 430 | -181.65911      | 770 | -228.95188      |
| 100 | -283.72214      | 440 | -182.82348      | 780 | -230.37653      |
| 110 | -263.02504      | 450 | -184.02312      | 790 | -231.79733      |
| 120 | -246.36339      | 460 | -185.25424      | 800 | -233.21416      |
| 130 | -232.79946      | 470 | -186.51371      | 810 | -234.62674      |
| 140 | -221.66341      | 480 | -187.79860      | 820 | -236.03501      |
| 150 | -212.46190      | 490 | -189.10612      | 830 | -237.43884      |
| 160 | -204.82491      | 500 | -190.43394      | 840 | -238.83807      |
| 170 | -198.46949      | 510 | -191.77977      | 850 | -240.23256      |
| 180 | -193.17513      | 520 | -193.14171      | 860 | -241.62224      |
| 190 | -188.76773      | 530 | -194.51772      | 870 | -243.00706      |
| 200 | -185.10821      | 540 | -195.90635      | 880 | -244.38690      |
| 210 | -182.08380      | 550 | -197.30588      | 890 | -245.76171      |
| 220 | -179.60241      | 560 | -198.71502      | 900 | -247.13138      |
| 230 | -177.58850      | 570 | -200.13240      | 910 | -248.49587      |
| 240 | -175.97860      | 580 | -201.55699      | 920 | -249.85516      |
| 250 | -174.71990      | 590 | -202.98752      | 930 | -251.20917      |
| 260 | -173.76784      | 600 | -204.42317      | 940 | -252.55790      |
| 270 | -173.08448      | 610 | -205.86289      | 950 | -253.90125      |
| 280 | -172.63716      | 620 | -207.30603      | 960 | -255.23923      |
| 290 | -172.39842      | 630 | -208.75166      | 970 | -256.57184      |
| 300 | -172.34390      | 640 | -210.19910      | 980 | -257.89903      |
| 310 | -172.45307      | 650 | -211.64778      | 990 | -259.22077      |
| 320 | -172.70755      | 660 | -213.09708      | 1000| -260.53710      |
| 330 | -173.09145      | 670 | -214.54644      | -   | -               |
| 340 | -173.59100      | 680 | -215.99539      | -   | -               |