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Energy harvesting using two-dimensional (2D) d-Silicates from abundant natural minerals

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Supporting information

Synthesis procedure

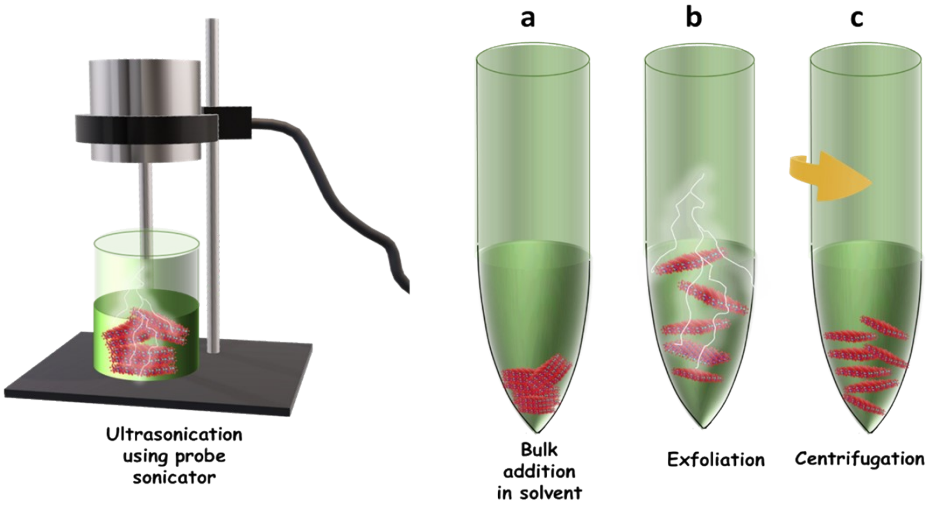

Fig. S1: Synthesis of 2D d-silicate via liquid phase exfoliation.

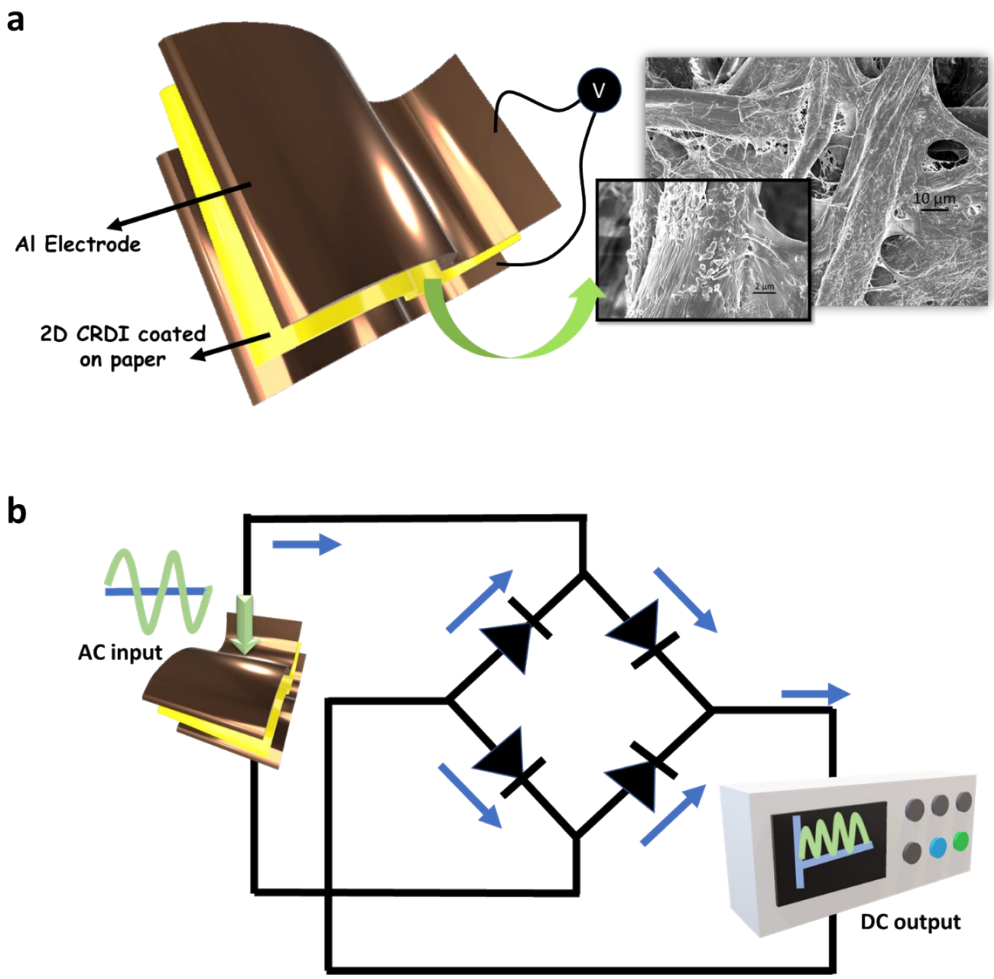

Fig. S2: Schematic of (a) fabrication design of flexible energy harvesting device with 2D d-silicate and SEM image of cellulose interaction with 2D d-silicate flakes, and (b) Bridge-rectifier circuit for converting AC voltage into pulsating DC voltage for use in power supplies.

Response measurement conditions:

Here the measurements were carried out at room temperature of about 307K, the force values varied from 0 to 5.88N. The device was kept on an insulated surface (paper sheet) and force was applied from one side of the device. The voltage output readings were recorded with a connected oscilloscope system. The noise value upon no load application was around 0.2V due to environmental factors. The signals are alternating positive and negative cycle sinusoidal waves due to the capacitor configuration. For application in DC devices where direct charging is required, a rectified electrical signal is needed. Mostly the AC to DC signal is achieved by employing a bridge rectifier circuit (as shown in Figure S2 (b)) where the signal can be rectified either to the positive or negative side.

Electron probe micro-analysis (EPMA)

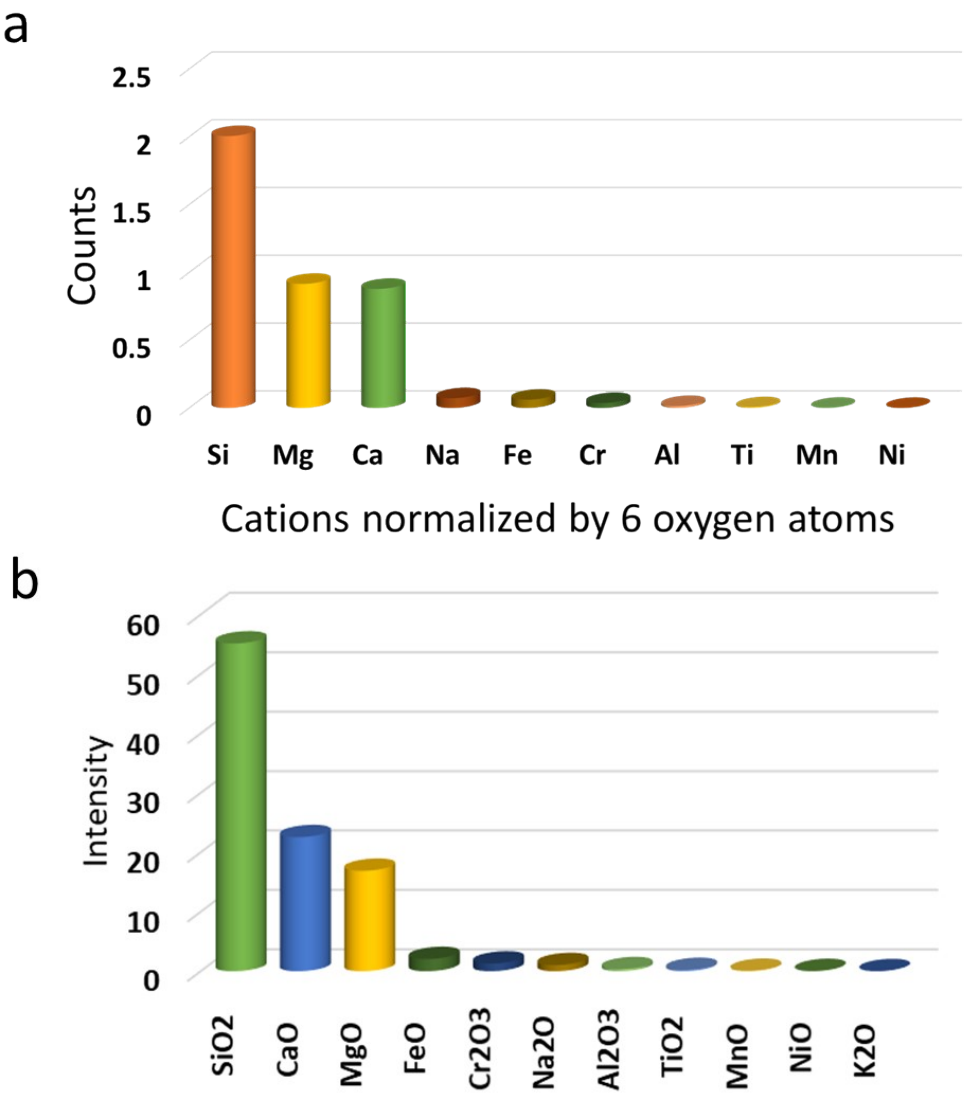

Fig. S3: (a) EPMA study of cations normalized by 6 oxygen atoms, and (b) EPMA quantification of oxide compounds in bulk diopside.

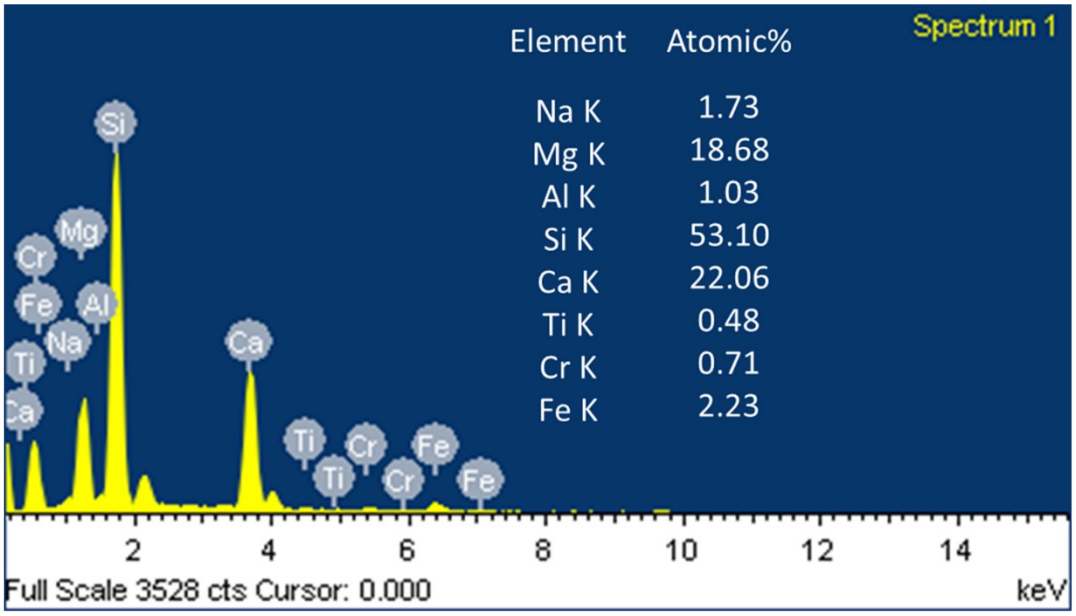

Fig. S4: EDX spectroscopy analysis showing atomic % of each element present.

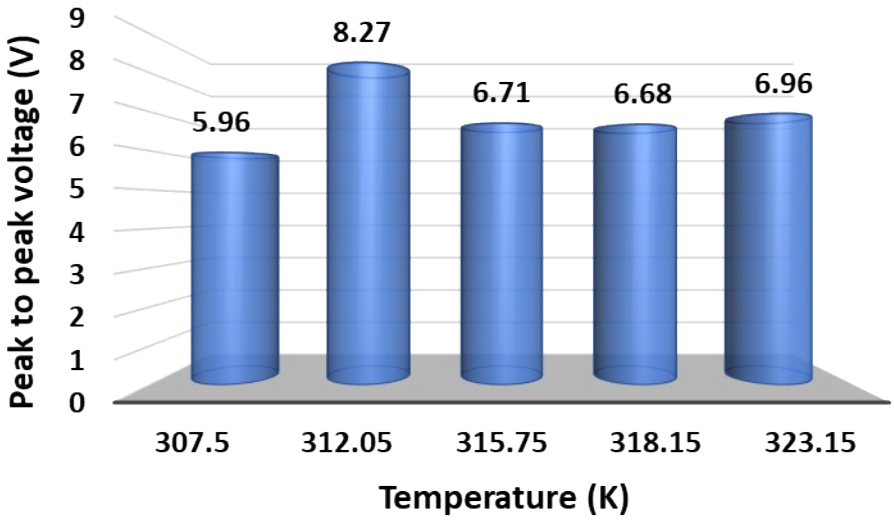

Fig. S5: Bar graph showing net peak-to-peak voltage output at various temperatures(K) with 0.98 N force.

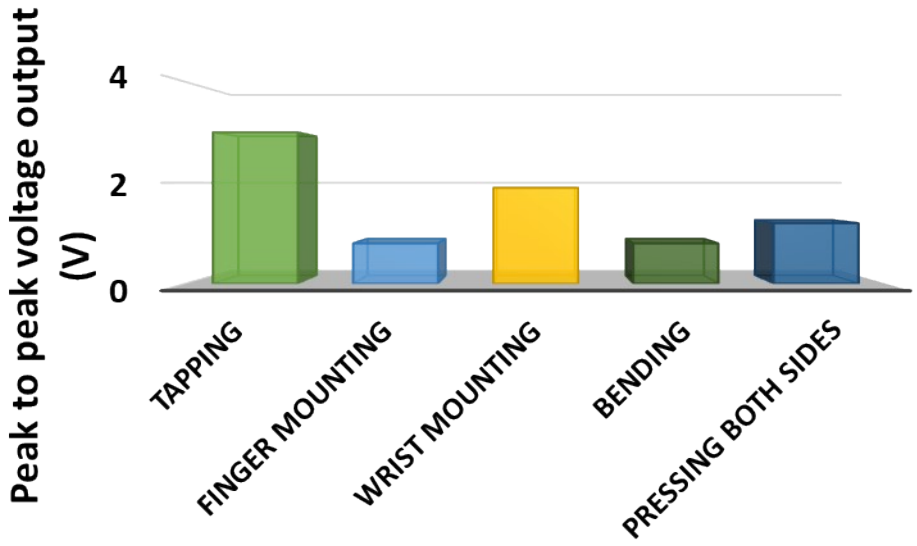

Fig. S6: Bar graph showing peak-to-peak voltage output for different physiological movements with the 2D d-silicate device.

DFT calculation details:

The measurement process and parameters for electrostatic potential:

The structure of the crystal planes and their orientation has a dependency on the work function values. The spatial distribution of the electrostatic potential in a vacuum was calculated far from the surface. Calculations were performed with the same settings applied during the variable cell relaxation. The results of the calculation are presented in Table 1 below.

Table-1: Anisotropy calculation summary for 2D *d*-silicate (1 au = 0.97 x 10^{22} V/m^2).

Atoms	V_{xx} [au]	V_{yy} [au]	V_{zz} [au]	η	Mulliken charges (e)
O	-0.358	0.2898	0.0682	0.2057	-1.23
Si	0.247	0.0228	-0.2698	0.6229	1.97
O	-0.3281	-0.1963	0.5244	0.3163	-1.21
O	0.5102	-0.3348	-0.1754	0.2926	-1.16
Si	0.3225	-0.5548	0.2323	0.2881	1.92
O	-0.3815	0.6316	-0.2501	0.2471	-1.10
O	-0.1479	0.5755	-0.4276	0.5522	-1.19
O	0.548	-0.2804	-0.2676	0.0226	-1.16

Si	0.2484	0.0185	-0.2669	0.632	1.97
O	-0.3577	0.297	0.0607	0.2046	-1.23
O	-0.3249	-0.2043	0.5292	0.296	-1.21
O	0.5103	-0.3371	-0.1732	0.2943	-1.17
Si	0.3207	-0.5515	0.2307	0.2874	1.92
O	-0.3854	0.6319	-0.2466	0.2472	-1.10
O	-0.1501	0.5762	-0.4261	0.5489	-1.19
O	0.5486	-0.281	-0.2676	0.0177	-1.16
Mg	0.0246	-0.1701	0.1455	0.5555	1.45
Ca	-0.1867	-0.2305	0.4172	0.3855	1.71
Mg	0.02	-0.165	0.1451	0.5973	1.45
Ca	-0.1812	-0.2363	0.4175	0.3664	1.71

The atomic information for the structural model is shown below:

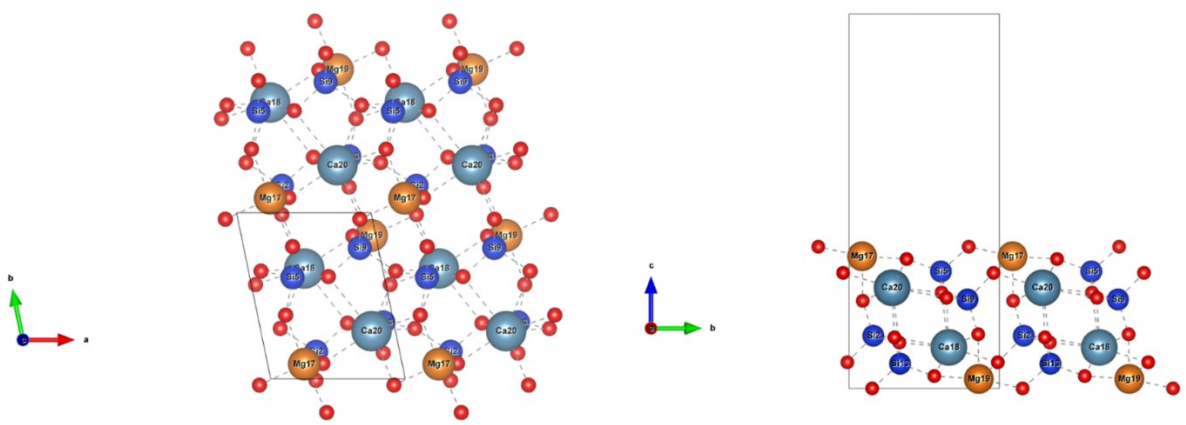

Figure R1*: 2D crystal structure of d-silicate, left and right view, used for DFT calculations.*

The structural formula is $ABSi_2O_6$, with A represented as $Ca_{0.89}Na_{0.073}Mg_{0.037}Mn_{0.002}$ in solid solution at the A site and $Mg_{0.879}Fe^{2+}_{0.062}Cr_{0.037}Al_{0.015}Ti_{0.006}Ni_{0.001}$ at the B site.

Lattice parameters

a	b	c	alpha	beta	gamma
9.69300	8.88900	5.25300	90.0000	106.3400	90.0000

Unit-cell volume = 434.323036 Å^3

Structural parameters

	x	y	z	Occ.	U	Site	Sym.

Mg	Mg1	0.00000	0.90680	0.25000	0.790	0.006	4e	2
Cr	Cr1	0.00000	0.90680	0.25000	0.090	0.006	4e	2
Al	Al1	0.00000	0.90680	0.25000	0.070	0.006	4e	2
Fe	Fe1	0.00000	0.90680	0.25000	0.050	0.006	4e	2
Ca	Ca2	0.00000	0.30080	0.25000	0.780	0.010	4e	2
Na	Na2	0.00000	0.30080	0.25000	0.180	0.010	4e	2
Mg	Mg2	0.00000	0.30080	0.25000	0.040	0.008	4e	2
Si	Si	0.28770	0.09270	0.23090	0.985	0.004	8f	1
Al	Al	0.28770	0.09270	0.23090	0.015	0.004	8f	1
O	O1	0.11500	0.08530	0.14050	1.000	0.008	8f	1
O	O2	0.36140	0.25190	0.31700	1.000	0.010	8f	1
O	O3	0.35130	0.01680	-0.00190	1.000	0.007	8f	1