

Supplementary Information

**NiO-Ti nanocomposites for contact electrification and energy harvesting:
Experimental and DFT+U studies**

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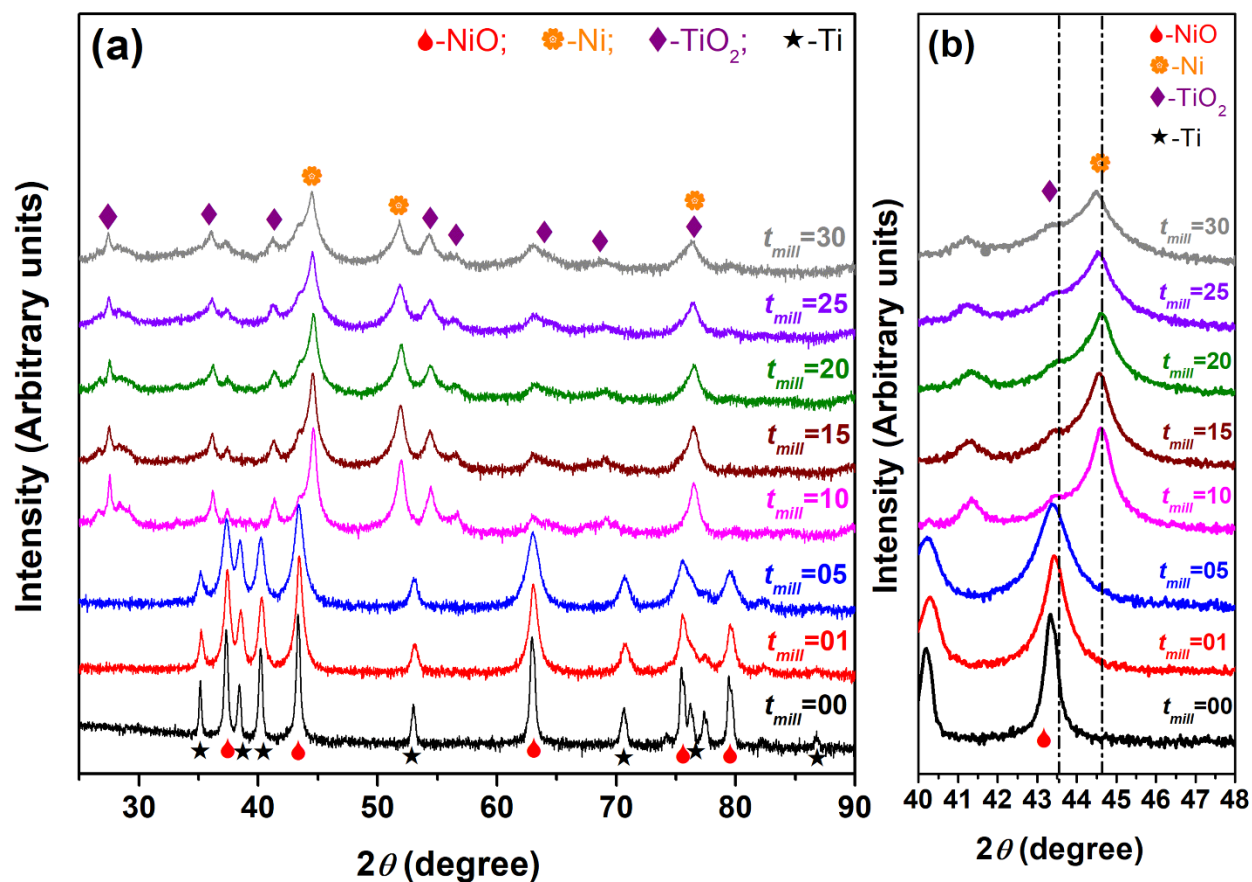


Figure S1: Milling time-dependent mechanochemical reduction of NiO by a reactive Ti to form an *in-situ* NiO-Ni-TiO₂ nanocomposite (a); The enlarged version of the peaks within $2\theta = 40\text{--}48^\circ$ showing the formation of Ni at the critical activation time of 10 h.

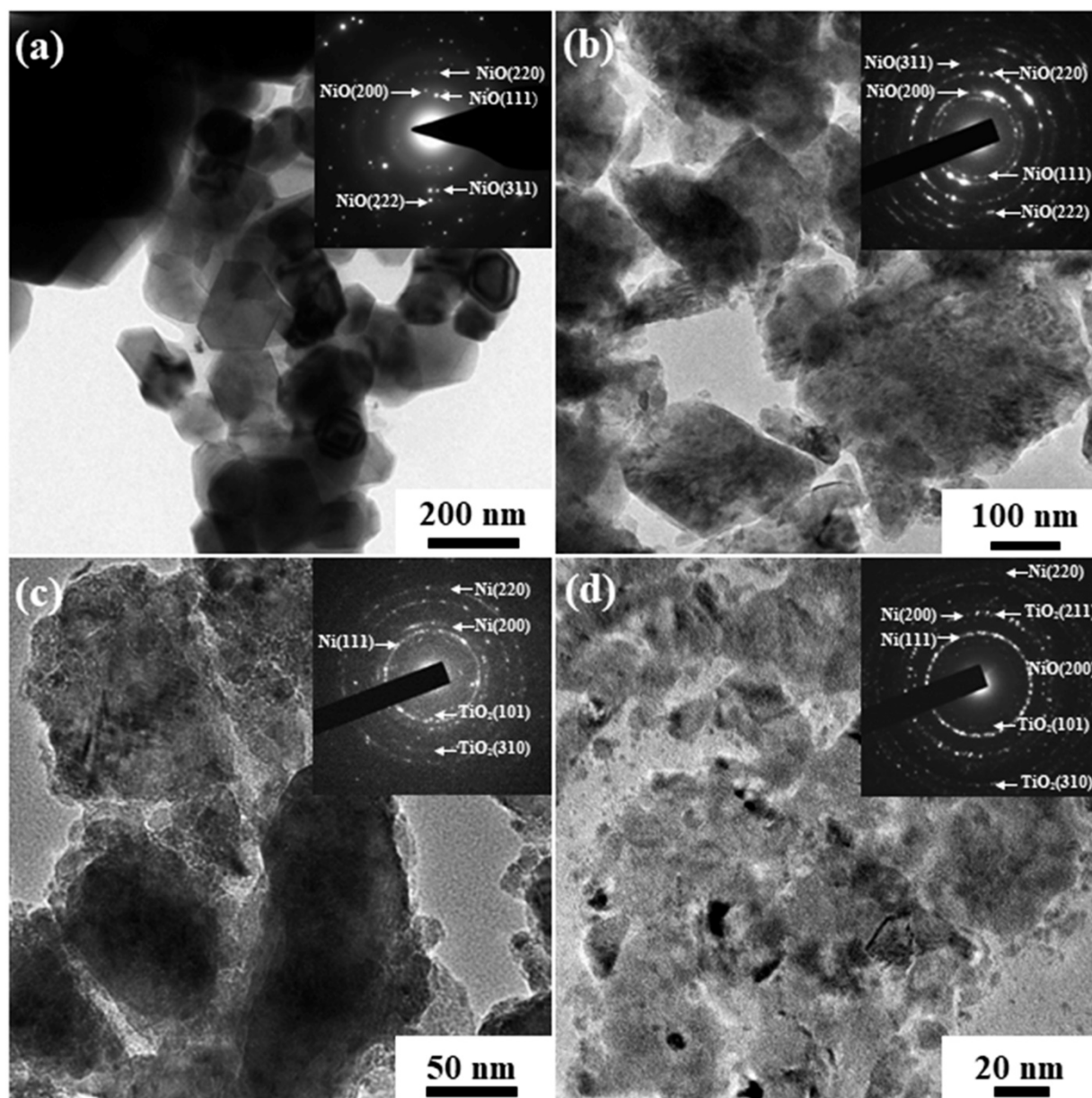


Figure S2: Bright-field TEM images and selected area electron diffraction patterns of NiO-Ti powders prepared at different milling periods with (a) Bulk NiO; (b) $t_{\text{mill}} = 5$ h; (c) $t_{\text{mill}} = 10$ h; (d) $t_{\text{mill}} = 30$ h.

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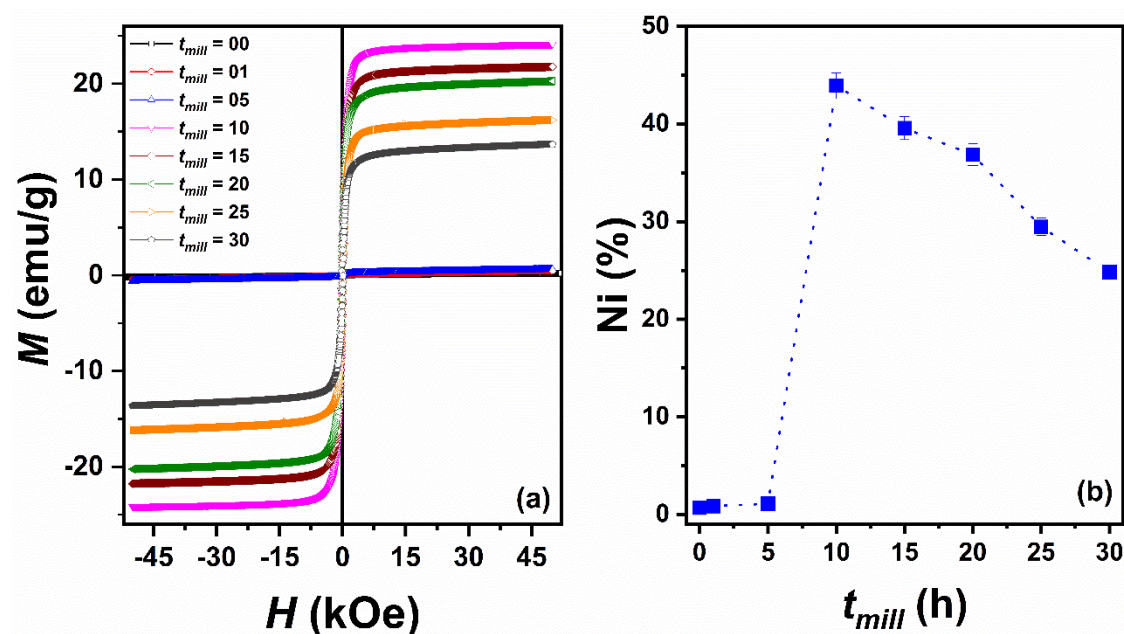


Figure S3: (a) Milling time-dependent magnetic hysteresis (M - H) loops measured at room temperature; (b) Percentage of Ni estimated for the NiO-Ti powders at different milling periods.

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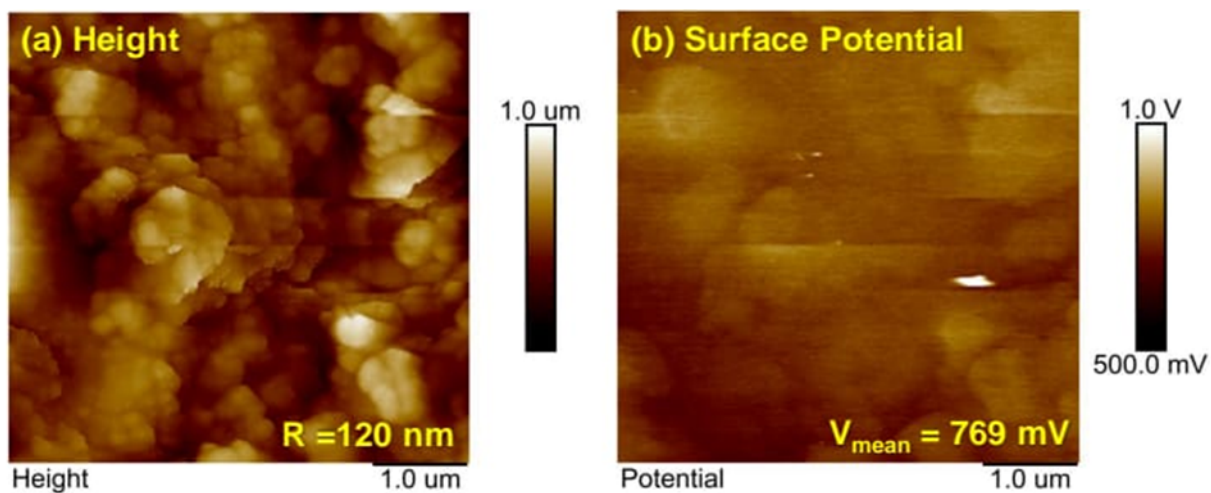


Figure S4: AFM (surface roughness) and KPFM (surface potential) features of the NiO-Ni-TiO₂ nanocomposite.

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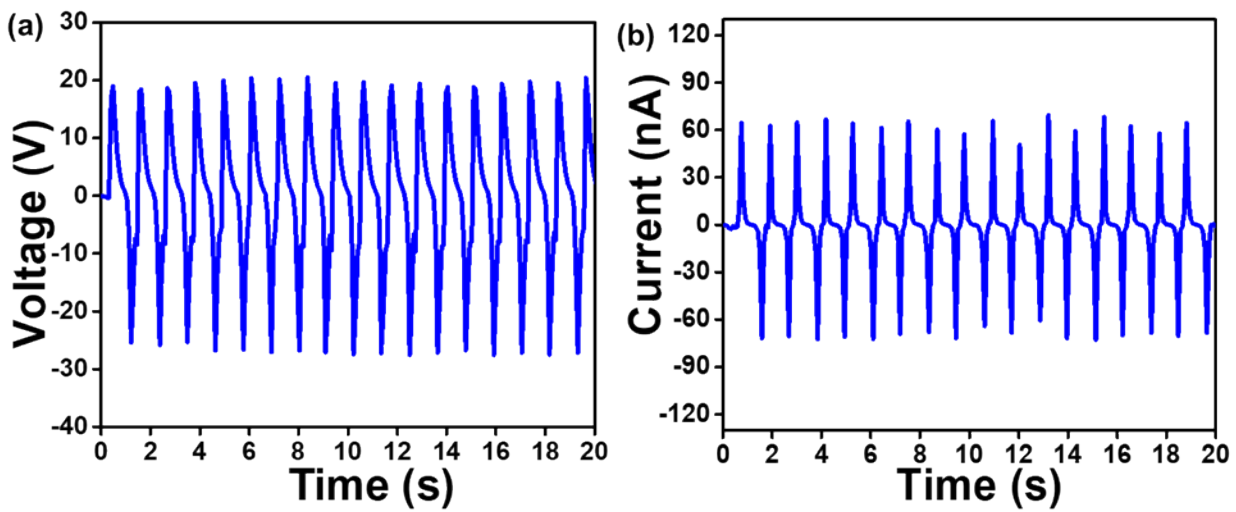


Figure S5: Voltage and current of the TENG based on NiO and Kapton triboelectric layers.

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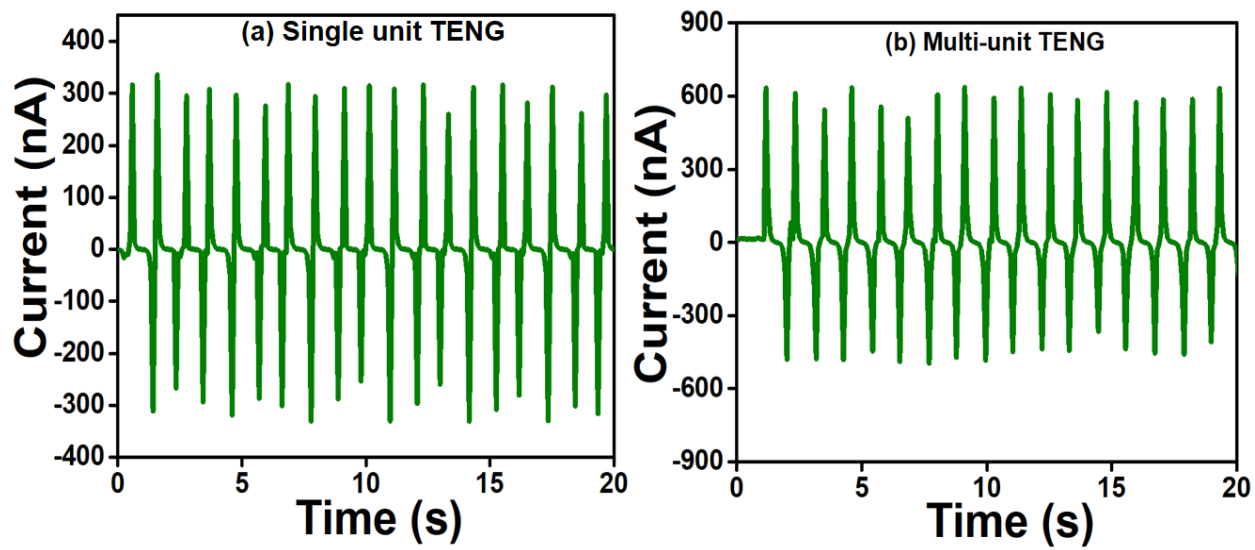


Figure S6: Electrical current output for single unit TENG and two units of TENG (multi) connected in parallel connection.

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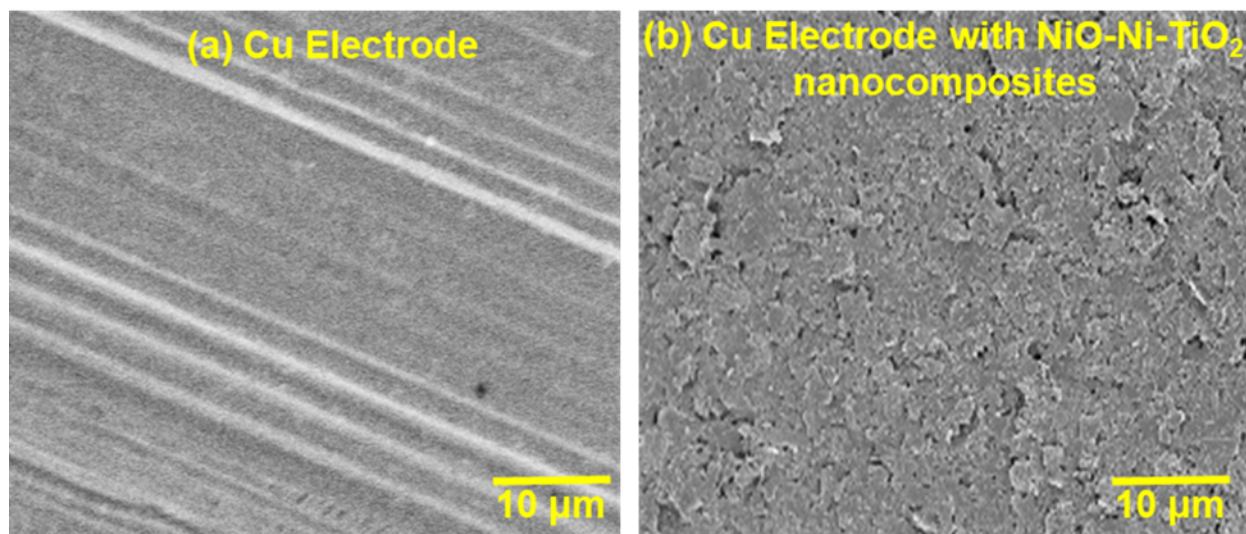


Figure S7: Surface micrographs of bare copper and NiO-Ni-TiO₂ particles attached to copper electrode.

Table S1: Comparison of different metal-oxide based TENG with present work.

Sl.	Device structure	Working Mode	Active Materials	Voltage (V)	Current (μ A)	Ref.
1	Spring Type Contact Separation	TENG	Kapton/ZnO	57	1.21	1
2	Spring Type Contact Separation	TENG-PENG hybrid	Ti _{0.8} O ₂ -Ag co-doped BaTiO ₃ /PDMS	150	0.32	2
3	Flapper type single electrode mode	TENG	ZnO nanorods/PDMS	5.34	0.181	3
4	Vertical contact mode	TENG	Ba ₃ Fe ₂ TeO ₉ /Kapton	88	2.69	4
5	Square shape vertical contact separation	TENG	Al ₂ O ₃ -PDMS	34	1.77	5
6	Square shape vertical contact separation	TENG	SiO ₂ -TiO ₂	0.2	-	6
7	Square shape vertical contact separation	TENG	TiO ₂ -HfO ₂	0.2	-	
8	Square shape vertical contact separation	TENG	Al ₂ O ₃ -HfO ₂	0.25	-	
9	Vertical contact separation	TENG	TiO ₂ -Natural rubber	45-78	4.5-7.0	7
10	Spring Type contact separation (2 cm $\times$ 2 cm)	TENG	NiO-Mg/Kapton	35	0.13	8
11	Spring Type contact separation (2 cm $\times$ 2 cm) two units in parallel	TENG	NiO-Mg/Kapton	35	0.49	
12	Spring Type contact separation (3.5 cm $\times$ 3.5 cm)	TENG	NiO-Mg/Kapton	80	1.0	
13	Eye-shaped vertical contact separation	TENG	NiO-Ni-TiO ₂ /Kapton	60	0.6	This work

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