

Abstract Submitted  
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**Single-layer honeycomb like structure of silica** SEYMUR CAHANGIROV, V. ONGUN OZCELIK, SALIM CIRACI, Bilkent Univ — Silica or  $\text{SiO}_2$ , the main constituent of earth's rocks has several 3D complex crystalline and amorphous phases, but it does not have a graphite like layered structure in 3D. Our theoretical analysis and numerical calculations from the first-principles predict that silica can have stable, suspended, single-layer honeycomb like allotrope,  $h\alpha$ -silica (silicatene), which can be viewed to be derived from the oxidation of silicene and it has intriguing atomic structure with re-entrant angles in hexagons. It is a wide band gap semiconductor, which attains remarkable electromechanical properties showing geometrical changes under external electric field. In particular, it is an auxetic nanomaterial with negative Poisson's ratio and has high piezoelectric coefficient. Coverage of foreign adatoms can attribute new functionalities to  $h\alpha$ -silica such that by oxidation it turns into to a wide band gap insulator like the parent quartz.

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