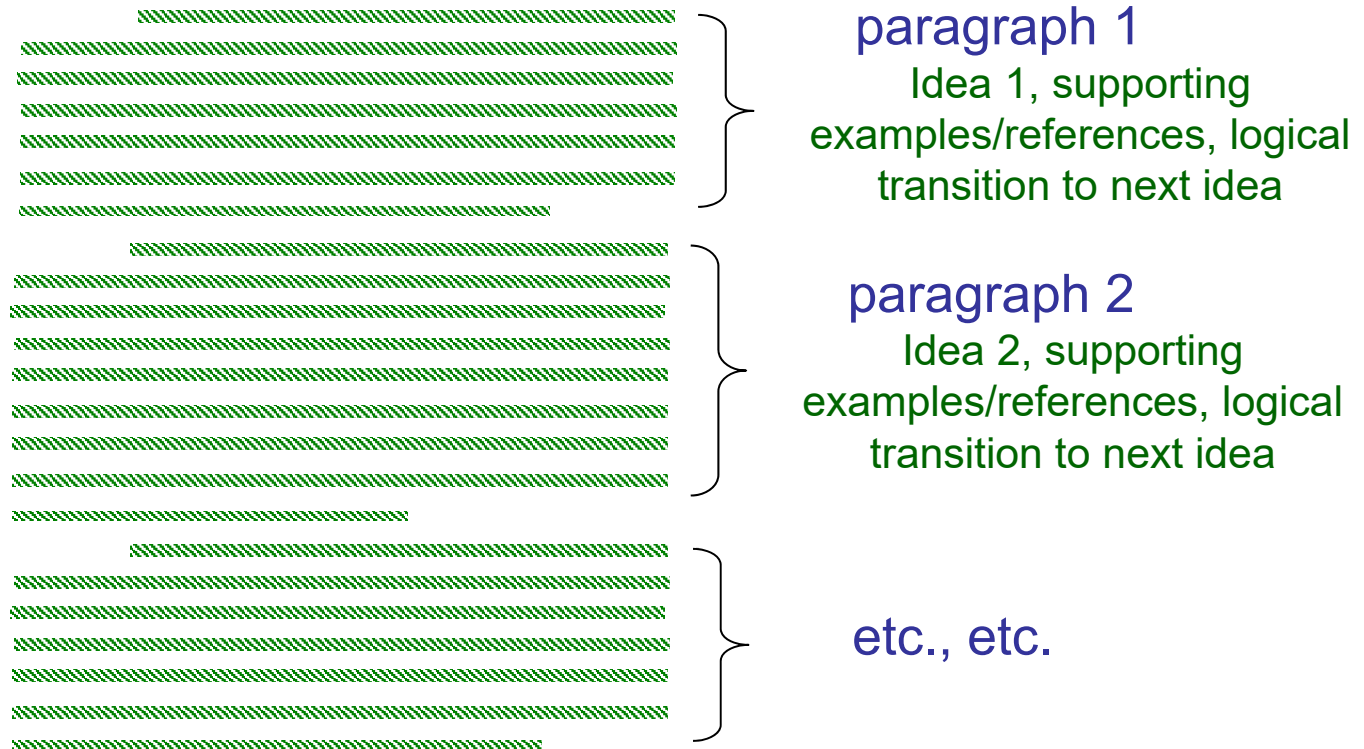


Things to keep in mind so that your scientific writing is logically structured, precise, and concise:

(1). Use paragraphs to maintain a logical structure

Every paragraph should contain roughly one idea + supporting evidence for that idea, if possible, and ***this idea should be presented as concisely as possible***



Writing Workshop #1: Paragraph Structure

The high-pressure and temperature phase transition of dioxides is of fundamental interest in solid-state physics, chemistry, and geosciences. In many dioxides, TiO_2 is well known as an important wide-gap oxide semiconductor with various industrial applications such as electrochemical solar cells and photocatalyst due to the characteristic high refractive index [1–9]. Apart from those technological aspects, high-pressure transformations of TiO_2 have attracted special attention as a low-pressure analog of SiO_2 , the most abundant component of the Earth's mantle. A number of experimental and theoretical studies have revealed many crystalline polymorphs of TiO_2 at high pressures and high temperatures [10–14]. At ambient conditions, rutile is the most stable phase of TiO_2 . Anatase and brookite are also known as natural minerals. All of these phases transform to an $\alpha\text{-PbO}_2$ -type, to an orthorhombic-I-type, then finally to a cotunnite-type structure at approximately 50 GPa [11,14]. The cotunnite-type polymorph is identified as the highest-pressure phase, as in many dioxides [15]. Although the analogy of the phase change to the cotunnite structure was applied to TiO_2 [16,17], a very recent *ab initio* study predicted a different phase transition from the pyrite-type structure to an unexpected Fe_2P -type structure (hexagonal, space group $P62m$) (Fig. 1) at 690 GPa, bypassing the cotunnite-type phase stability at low temperature [18]. Since no dioxides or difluorides with this crystal structure were reported, physical and chemical properties of this new class of oxide are still unknown. Although the extremely high transition pressure predicted in SiO_2 seems unreachable in the laboratory, TiO_2 shows significantly lower transition pressures. For instance, the $\alpha\text{-PbO}_2$ phase stabilizes at ~ 10 GPa in TiO_2 , while the same phase at 100 GPa in SiO_2 . High-pressure behavior of TiO_2 is therefore a key to understanding the rich polymorphism in the metal dioxide systems, in particular, the post-cotunnite phase relations. However, all the studies performed on TiO_2 were limited below 100 GPa, and no post-cotunnite phase has been identified. In this study, we investigate the applicability of the Fe_2P -type structure to TiO_2 .

Topic sentences

The high-pressure and -temperature phase transitions of dioxides are of fundamental interest in solid-state physics, chemistry, and the geosciences. In particular, because of its high refractive index [1-9], TiO_2 is an important wide-gap oxide semiconductor for various industrial applications, such as electrochemical solar cells and photocatalysts. Additionally, high-pressure transformations of TiO_2 have attracted special attention as a low-pressure analog of SiO_2 , the most abundant component of the Earth's mantle.

Previous experimental and theoretical studies reveal many crystalline polymorphs of TiO_2 at high pressures and high temperatures [10–14]. Rutile is the most stable phase of TiO_2 at ambient conditions, but TiO_2 exhibits a structural phase transition from orthorhombic-I-type to cotunnite-type structures at approximately 50 GPa [11,14]. Cotunnite was previously reported to be the highest pressure phase of TiO_2 [15]. However, a recent *ab initio* study of TiO_2 predicted a transition from the pyrite-type structure to an Fe_2P -type structure (hexagonal, space group $P62m$) (Fig. 1) at 690 GPa. This transition bypasses the cotunnite-type phase stability at low temperatures [18]. Unfortunately, because no dioxides or difluorides with the high pressure Fe_2P -type crystal structure have been reported, the physical and chemical properties of the high pressure structural phase of oxides are still unknown.

Studying the high-pressure structural phases of TiO_2 is key to understanding the rich polymorphism in the metal dioxide systems. TiO_2 exhibits significantly lower transition pressures to post-cotunnite phases than other dioxides. For instance, the α - PbO_2 phase stabilizes at ~ 10 GPa in TiO_2 , while the same phase stabilizes at 100 GPa in SiO_2 . However, all the studies performed on TiO_2 have been limited to 100 GPa, and as yet no post-cotunnite phases have been identified. In this study, we theoretically and experimentally investigate the high pressure structural phases of TiO_2 , in particular to determine if this material exhibits a Fe_2P -type structure at high pressures.

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Transition sentences

Previous experimental and theoretical studies reveal many crystalline polymorphs of TiO_2 at high pressures and high temperatures [10–14]. Rutile is the most stable phase of TiO_2 at ambient conditions, but TiO_2 exhibits a structural phase transition from orthorhombic-I-type to cotunnite-type structures at approximately 50 GPa [11,14]. Cotunnite was previously reported to be the highest pressure phase of TiO_2 [15]. However, a recent *ab initio* study of TiO_2 predicted a transition from the pyrite-type structure to an Fe_2P -type structure (hexagonal, space group $P62m$) (Fig. 1) at 690 GPa. This transition bypasses the cotunnite-type phase stability at low temperatures [18]. Unfortunately, because no dioxides or difluorides with the high pressure Fe_2P -type crystal structure have been reported, the physical and chemical properties of the high pressure structural phase of oxides are still unknown.

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