

Scientific Plausibility Flags in PEM Catalyst Patents

Inflexion Report excerpt · Green Hydrogen / PEM Electrolysers · April 2026

Executive Briefing

Cross-referencing PEM electrolyser catalyst patents against Materials Project thermodynamic data reveals a consistent pattern: patents claiming novel IrO₂ polymorphs or MoS₂/WS₂-based catalysts for acid PEM service frequently omit phase stability data that would determine whether the claimed material can survive operating conditions. Two implausibility flags are identified in this excerpt.

IrO₂ Polymorph Analysis — Patent Plausibility Matrix

Phase	MP ID	E _{hull} (eV/atom)	Assessment	Patent Signal
Rutile IrO ₂	mp-2723	0.000 (stable)	Validated	Dense prior art. Limited white space.
Cubic IrO ₂	mp-1095353	0.076	White Space	Metastable — filing opportunity if synthesis route claimed.
Tetragonal IrO ₂	mp-1014261	0.263	Flag	High instability — patents claiming stable operation are implausible.
Rutile RuO ₂ (comparator)	mp-825	0.000 (stable)	Validated	Strong prior art; iridium supply risk drives substitution research.

Source: Materials Project. E_{hull} values from DFT calculations. Density of rutile IrO₂: 11.548 g/cm³; cubic IrO₂: 12.633 g/cm³.

Implausibility Flag #5: MoS₂/WS₂ for Acid PEM Service

■ IMPLAUSIBILITY FLAG — MATERIAL-ENVIRONMENT MISMATCH

Several patent families claim MoS₂ or WS₂ as anode catalyst materials for PEM electrolyzers. Materials Project data shows MoS₂ is a semiconductor (band gap 1.2 eV) with a tetragonal phase sitting 0.648 eV/atom above the convex hull — indicating severe metastability. More critically, both materials dissolve rapidly under the strongly acidic conditions (pH < 1, 80°C+) of a PEM anode. Independent literature confirms MoS₂ and WS₂ are not viable under these conditions without extraordinary stabilisation measures. Patents claiming durable PEM anode performance from these materials without acid-stability data are scientifically implausible.

Band gap MoS₂: 1.2 eV (semiconductor, not metallic conductor needed for electrocatalysis) · Band gap WS₂: 1.6 eV · MoS₂ tetragonal phase E_{hull}: 0.648 eV/atom

■ **White Space Identified: Cubic IrO₂ (mp-1095353) — metastable polymorph with 12.633 g/cm³ density (8.5% denser than rutile). High surface area potential. Synthesis route claims remain largely unpatented. Opportunity window estimated: 12 – 24 months before major assignees file.**

The full Green Hydrogen Inflexion Report covers 80+ patents across IrO₂, RuO₂, and transition metal alternatives — with iridium supply chain risk analysis and an R&D investment prioritisation matrix.

Full Inflexion Report: £2,500 · 50–70 pages · 2–3 week delivery