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## Computational studies of the corrosion mechanisms in transformers

The failures of transformers have been linked to the interaction of copper sulphide with copper windings. The copper sulphide is a product of copper particles that react with the corrosive sulphur within the transformer oil. This copper sulphide thereafter deposits on the vacant sites of the copper windings [1, 2].

Our research focuses on the interaction of copper sulphide on various copper surfaces. This interaction represents the corrosion of the copper windings. The molecules involved in the reaction mechanism were model using the Perdew-Burke-Ernzerhof (PBE) Generalized Gradient Approximation GGA functional which describes the exchange correlation functional. First principles calculations were based on an optimized copper bulk structure and the copper surface. The energetic and electronic properties of the lowest interaction configurations were analyzed.

### HPC Content

This study used the Materials Studio 2018 software on the Lengua Cluster at the Centre for High Performance Computing (CHPC). The softwares CASTEP and DMOL3 Modules were used to compare different methods of the adsorption of copper sulphide on different copper surface.

[1] Lewand L R, The role of corrosive sulphur transformers and transformer oil, Proc 69th Annual Int Conf Doble Clients (Doble Engineering, Boston) 2002.

[2] Tanimura J, Toyama S, Kawarain H, Mizuno K, Hosokawa, Kato F & Amimoto T, Development of diagnostics to estimate the risk of copper sulfide formation for transformers, Proc 77th Int conf Doble Client ( Doble Engineering, Boston) 2010.

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