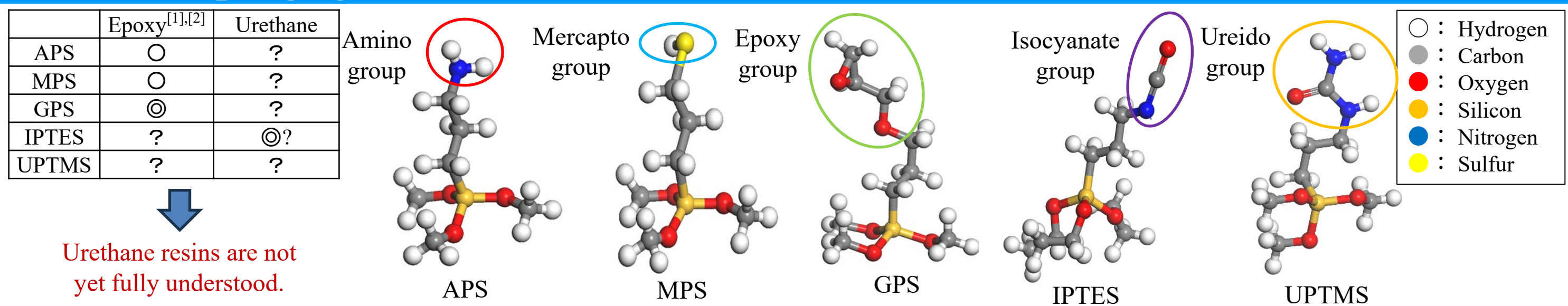


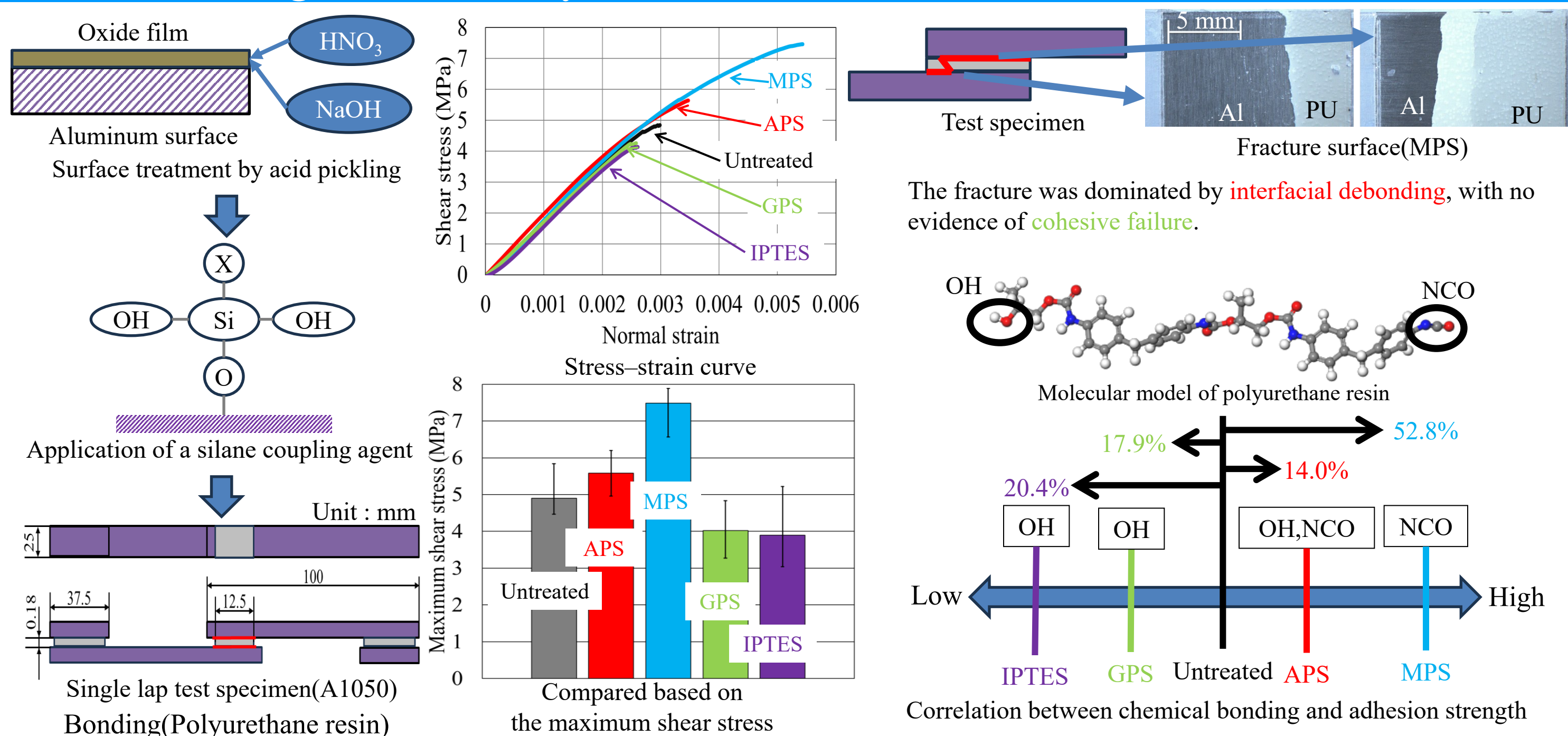
Introduction

Multimaterial design aimed at weight reduction and performance enhancement has become increasingly prevalent across a wide range of fields, from automotive to medical devices. In particular, the adhesion between metals and plastics requires the formation of strong chemical bonds between inorganic and organic materials, for which **silane coupling agents (SCAs)** are commonly employed. To appropriately select SCAs for a given material combination, it is essential to elucidate, at the atomic scale, the interfacial bonding states as well as the molecular deformation and mechanical responses under load, in order to understand their influence on macroscopic adhesion strength. In this study, the effect was evaluated through tensile shear tests and first-principles calculations.

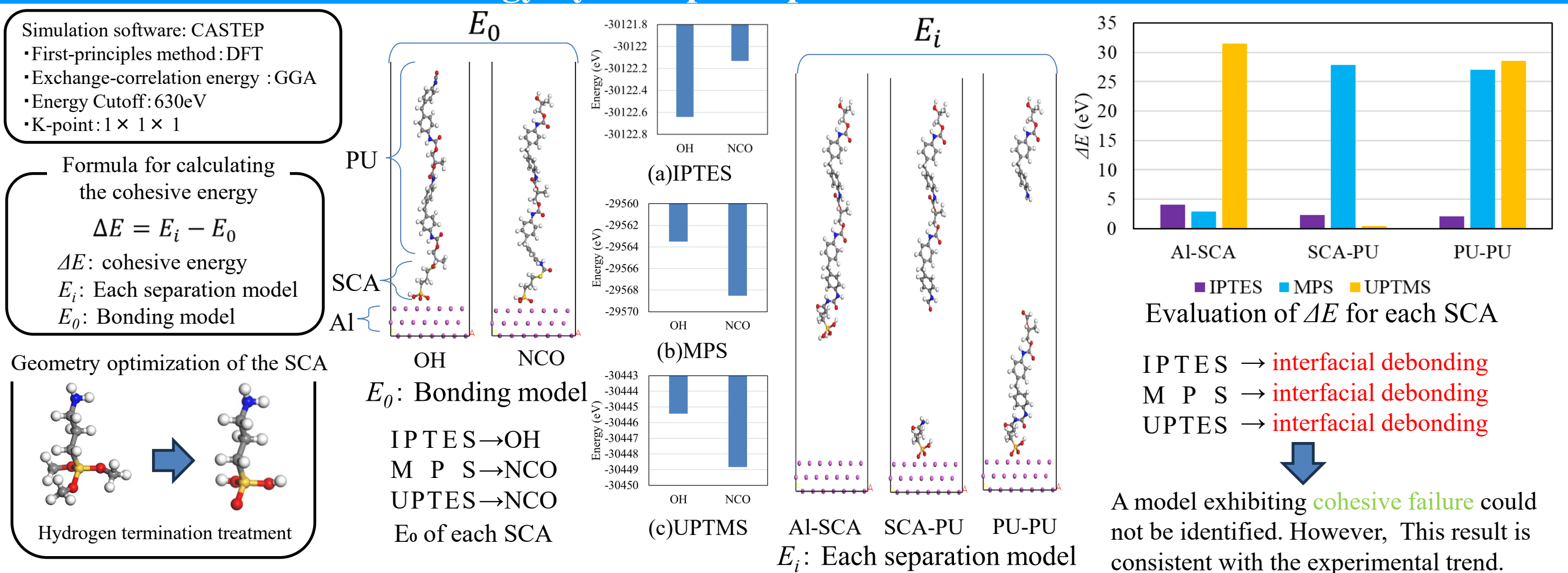
Silane coupling agents



Adhesive strength evaluation by tensile shear test



Evaluation of cohesive energy by first-principles calculations



[1] Uetsuji Y., Fukui N., Yagi T., Nakamura Y., Journal of Materials Research, 37 (2022) 923-932.

[2] Fukui N, Okunishi T, Hara N, Nakamura Y, Uetsuji Y., International Journal of Mechanical Sciences, 246 (2023) 108150.