

Energy Inversion Principle (EIP), reconstructing molecular binding energy via input-output energy differentials

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1 Introduction

Molecular binding energy is a fundamental quantity that determines the structural stability, reactivity, and thermodynamic behavior of matter across physics, chemistry, and engineering domains. However, direct quantification of binding energy, especially in gas-phase systems, has remained highly challenging. Traditional measurement techniques often depend on cryogenic conditions, spectrometric equipment, or indirect energy state inference, making them expensive, inaccessible, or sensitive to system conditions.

In this work, we propose the **Energy Inversion Principle (EIP)**, a physically grounded analytical method for **reconstructing molecular binding energy via input-output energy differentials** under a pressure-induced experiment. By applying a known amount of input energy E_{in} and measuring the emergent output energy E_{out} , we define the absorbed energy, equivalent to the total binding energy E_b , as:

$$E_b = E_{\text{abs}} = E_{\text{in}} - E_{\text{out}}$$

For mixed gas systems with known molar fractions x_i , this generalizes to:

$$E_{\text{abs}} = \sum_{i=1}^n x_i \cdot E_{b_i}$$

where E_{b_i} denotes the molecular binding energy associated with species i .

Importantly, if x_i is unknown and a non-zero residual is detected through

$$E_{\text{residual}} = E_{\text{in}} - E_{\text{out}} - \sum_{i=1}^n x_i E_{b_i},$$

this residual implies the existence of unaccounted gas components. Thus, the EIP acts as a dual-purpose system: a **binding energy reconstruction tool** and a **hidden component detector**.

This paper presents the theoretical formulation of EIP, experimental setup requirements, reconstruction procedures, and potential applications in gas analysis, CO₂ monitoring, and reactive system characterization.

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