個人情報

受賞

1） International Conference of Computational Methods in Science and Engineering (ICCSSE) 賞 （2006年）

2） 日本化学会学会賞 （2007年）

3) European Society of Computational Methods in Science and Engineering (ESCMSE) 欧州学会賞 （2008年）

研究費

1)（科研）基盤研究（B） 平成18年度―平成20年度

2)（科研）基盤研究（C） 平成21年度−平成23年度

職歴

1） 大阪大学極限量子科学研究センター
特任教授 平成19年度―20年度

2） 大阪大学ナノマテリアルデザイン教育研究センター
招聘教授 平成21年度

その他

1) 新学術領域研究「配位プログラム」評価委員

研究成果

本研究は電子間反発相互作用が強く、その効果が無視できない多電子系（強相関電子系）の量子化学基礎理論の開発から始めて、化学反応、分子物性、生体分子システムへとその理論展開を実行したものである。 研究対象の多様性にもかかわらず、研究内容は強相関電子系、対称性の破れ、3つの自由度（軌道、スピン、電荷）などのキーワードにより相互に深く関連した内容になっている。このことは1970年代に開発した基礎理論が幸運にも適用領域が広範であったことと関連分野の実験が爆発的に発展したを反映している。以下に各分野の研究成果の概要について述べる。

I) 量子化学基礎理論

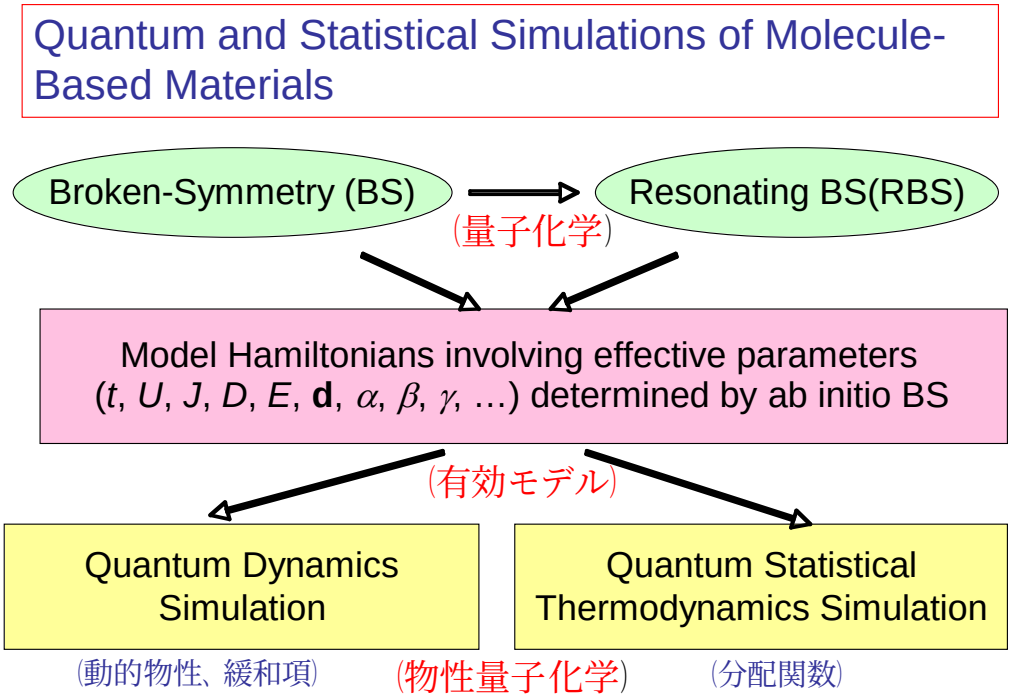
電子間相互作用の強い多電子系（強相関電子系）の電子状態理論および化学結合理論を構築した。 特に今日「対称性の破れ」（Broken-Symmetry (BS)）の方法と総称される基礎理論を開発し、その根源にある静的電子相関およびスピン相関の重要性を解明した。 また、BS 解の共鳴を考慮することにより分子軌道理論（Molecular Orbital (MO) Theory）と原子価結合理論(Valence Bond (VB) Theory) の統合にも成功した（原著論文 12,13,45、英文総説 3,13,20）。さらに、BS 解の自然軌道解析を行い、その占有数に基づき静的電子相関に対応する活性軌道空間（CAS）を選択し、残りの動的電子相関を配置間相互作用（CI），多体摂動論（PT），結合クラスター（CC）法で求める道筋を開拓した。これらの基礎理論の信頼性、有効性、その他を以下に述べる各分野の現象、例えば磁気的相互作用(J)の理論計算など、に適用し数多くの実験結果と比較することにより実証した（原著論文 46,51）。

II) 反応量子化学

電子間反発相互作用が強く電子が局在化し局在スピンが出現する系に適用可能なスピンハミルトニアン（ハイゼンベルグ）モデルを用いてラジカル反応の磁性群論的選択則を導出した（原著論文 10,14,33）。化学反応機構を独立粒子モデルに立脚して理論的に把握するための概念として「対称性の破れ」(BS)を導入し、「対称性の保存」の概念と組み合わせることにより、協奏反応、双極イオン反応、ビラジカル反応およびイオンラジカル反応を統一的に解析可能な反応理論を構築した。 また、BS MO 計算により得られる電荷およびスピン密度分布と上記反応の分類は1：1に対応することを示した。特に酸素化反応に同理論を展開し、基質特異性、反応場の変化などにより反応系の軌道、スピン、電荷の自由度が如何に転換しうるかを解明し、上記反応機構の動的変換過程を明らかにし、外場による反応制御の可能性を実験家と共同で検討した（原著論文 6,7,8,英文総説 1,2,4）。

III) 物性量子化学

分子をボトムアップ的に集積化して分子集合系（メゾスコピック系）や分子固体（無限系）を形成した場合の物性発現の可能性や理論的解析を実行する量子化学分野を,1980以降の物性化学の膨大な実験結果の集積を背景に,「物性量子化学」という新学問領域として体系化した。特に、強相関電子系の特徴であるスピンを持つ分子間の磁気的相互作用の理論計算から始めて、超常磁性、分子磁性体（長距離秩序）の形成による磁性発現の機構を量子力学と統計力学を連結する多階層連結計算手法により解析した。また、スピン相関やスピンフラストレーションの強い系の量子化学計算に基づき銅酸化物と等電子的物質系の分子設計を行い分子磁性金属、有機近藤系、スピン揺らぎ高温超伝導体の分子設計にも展開した。さらに、強相関電子系の励起状態（光）物性、特に非線形光学現象や励起子の動的挙動の理論的解析を実行した。なお、スピンおよび擬スピンモデルを構築し、磁性、超伝導、量子光学、原子光学分野を統一的に把握し、等価変換的視点より新規物質の分子設計を実行した（原著論文 70,90,99,105,110,英文総説 5-12,英文本1、日本語本2、日本語総説 25-27,29）。

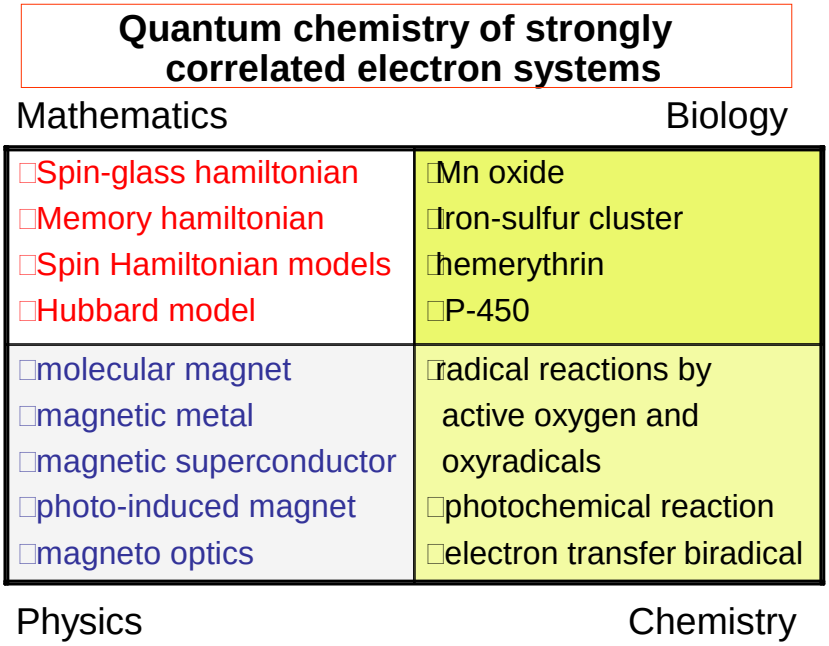


説明図 1　**物性量子化学の基礎理論**

IV)　生体機能量子化学

生体内酸化還元酵素系では、強相関電子系の典型例と見なされるマンガン多核錯体や鉄—イオウ多核錯体が活性中心を形成している場合が多い。従って、これらの酵素系は強相関電子系を蛋白場により閉じ込めて(confinement)その機能発現を制御している複合分子システムと見なすことが可能である。この視点より分子システムの動作機構の解明を目指してまず構成部品である上記クラスターの電子構造と化学結合様式を解明し、その特性が水素結合などの蛋白場によりどのように変動しうるかを解明した。例えば、基底三重項状態にある酸素分子が、生体内酸素化反応過程において基質との電子移動とスピン軌道相互作用を媒介にして一重項に変換される機構を解明した。其の次のステップとして構成部品間の相互作用を考慮し分子システムとしての動作機構を QM/MM/MD 法により解明する研究を現在進めている（原著論文 63,65,79,94,97102,英文総説 2,4）。これらの研究を最終的には「生体機能量子化学」として集大成することを本研究所での研究目標にしている。

本研究で開発した基礎理論の適用領域を纏めると図2のようになる。



説明図2　強相関電子系の適用領域

Publication List of Professor Kizashi Yamaguchi

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