学会及び社会における活動等

１９６６．４　日本物理学会会員（現在に至る）
１９８８．４　米国物理学会会員（２００６．３まで）
１９８８．４　ヨーロッパ物理学会会員（２００６．３まで）
１９８８．４　「第７回液体とアモルファスに関する国際会議」組織委員（1989 年 9 月まで）
１９８８．４　「第 26 回山田国際会議（強結合プラズマ物理）」組織委員（1989 年 9 月まで）
１９８９．４　「第 13 回谷口国際シンポジウム（分子動力学シミュレーション）」組織委員（1990 年 11 月まで）
１９９０．４　科学技術庁「計算科学に関する調査研究」推進委員（1992 年 3 月まで）
１９９０．４　「第１回東和大学国際会議（凝縮系におけるスローダイナミックス）」組織委員（1991 年 11 月まで）
１９９１．４　「第 6 回分子シミュレーション討論会」実行委員長（1992 年 11 月まで）
１９９４．４　「第１回東和大学交際会議（理論、実験、計算機シミュレーション）」組織委員（1995 年 11 月まで）
１９９４．４　東京大学物性研究所スーパーコンピュータ共同利用運営委員会委員（1996 年 3 月まで）
１９９５．４　日本原子力研究所原子力研究委員会委員、同専門部会長（1995 年～2000 年、2000 年～2006 年）
１９９６．４　日本計算工学会会員（2006 年 3 月まで）
１９９６．４　東京大学物性研究所スーパーコンピュータ共同利用運営委員会委員（2002 年 3 月まで）
１９９６．11　湯川記念国際シンポジウム主催（京都市）
１９９７．４　東京大学物性研究所運営委員（2001 年 3 月まで）
１９９７．11　日本分子シミュレーション研究会会長（2004 年 11 月まで）
１９９９．４　日本化学技術戦略推進機構計算科学部会会員（2001 年 3 月まで）
１９９９．11　計算物理学国際会議主催（金沢市）
２０００．４　東京大学物性研究所外部評価委員（2001 年 3 月まで）
２０００．４　金沢こども科学財団評議員（2002 年 3 月まで）
２００２．４　岡崎研究機構分子科学研究所外部評価委員（2003 年 3 月まで）
２００３．４　文部科学省超高速コンピュータ網形成プロジェクト（NAREGI）
ナノグリッド自己評価委員（現在に至る）
２００４．１　分子シミュレーション国際会議主催（つくば市）
２００４．４　石川県教育委員会・スーパーサイエンスハイスクール運営委員会委員長（2006 年 3 月まで）
２００４．４　独立行政法人産業技術総合研究所研究ユニット評価委員（2006 年 3 月まで）
２００４．４　岡崎研究機構分子科学研究所外部評価委員（現在に至る）
２００４．６　石川県教育委員会小学校科学実験サポータ（2006 年 3 月まで）

２００４．９　虎姫高等学校出張講義
２００４．11　七尾高等学校出張講義
２００５．３　(独) 海洋研究開発機構地球シミュレータ研究センター外部評価委員（2006.3 まで）
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２００５．10　平成１７年度金沢大学公開講座「親・子・教師向けサイエンストーク」主催
２００５．10　全国高等学校理数科大会総合講演（招待講演）
２００６．１　(理化学研究所) 次世代スーパーコンピュータ・開発戦略委員会・
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次世代スーパーコンピュータ共用ワーキンググループ委員（2007 年 3 月まで）
２００６．６　NPO 法人いしかわサイエンス 21　理事長に就任（現在に至る）
２００６．４　金沢大学大学院自然科学研究科および理学部非常勤講師（2007 年 3 月まで）
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２００７．４　金沢大学大学院自然科学研究科および理学部非常勤講師（現在に至る）
２００７．９　文部科学省（石川県）主催小学校理科支援事業特別講師（現在に至る）
２００７．10　日本物理学会誌アルダー転移５０周年特集号編集（企画委員長）
２００７．11　平成１９年度金沢大学公開講座「サイエンストーク」担当講師
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科学研究費と外部資金受入れ情報

科学研究費補助金

(1) 基盤研究C、平成15年度～平成16年度、「高分子動的誘電特性の分子動力学シミュレーション」、研究代表者、3,600千円、研究成果(概要):

(i) PPO [Poly (2, 6 - dimethyl - 1, 4 - phenylene oxide)] の粗視化モデルを考察し、分子動力学シミュレーションにより、PPOの動的誘電特性, 複素誘電率、コール・コールプロットなどからPPO高分子内のフェニレン基と酸素を結ぶ結合の偏角振動モードと誘電特性を明らかにした。(ii) ポリマーの基本的な性質(ガラス転移温度、熱膨張係数、比熱など)の支配要因(ミクロパラメーター)を自由に制御する支配要因を探すことを目的に、ナノコンポジット系の分子動力学シミュレーションを行った。ポリマー(PE)にナノサイズの粒子を加えることによる物性(特にガラス転移温度)の変化を考察した。

科学研究費補助金以外

(1) NEDO, 平成8年～平成10年,「高分子・分子集合体の自由エネルギーの計算法と超高速専用計算デバイスの開発」、研究代表者、89,000千円、研究成果(概要):

本研究においてクーロン相互作用を含む高分子系の自由エネルギー計算を効率かつ精度良く計算する計算アルゴリズムおよび計算システム(専用並列計算システム)を開発した。

(2) JST, 平成10年～平成13年,「高分子会合(秩序)・解離(無秩序)の分子論的研究」、研究代表者、152,200千円、研究成果(概要):

本プロジェクト研究は、会合・解離の分子理論的考察を始め、分子シミュレーションによる会合模擬実験を通して分子レベルの会合に関する新しい知見(例えば疎水的会合などの分子論)や種々の高分子系(蛋白質など)の構造変化(会合・解離)の特質を相互作用の型およびその大きさにより解明を試みたものであり、これにより分子設計への道標を示唆するものである。

(3) 日本原子力研究所、平成10年～平成12年、「分子シミュレーションにおける並列計算技法の開発と応用」、研究代表者、24,840千円、研究成果(概要):

本研究により、古典粒子系の分子動力学シミュレーション・コードの並列化および電子系タイトバインディングモデルの並列化計算コードの開発研究ななどを行なった。また、これらの分子動力学シミュレーション・コードを興味ある物理・化学系に適用を試みた。

(4) 通信・放送機構、平成12年～平成14年、「ギガビットネットワークを利用した広域仮想シミュレーション工場の提案」、研究代表者、60,000千円、研究成果(概要):

仮想シミュレーションラボの基盤構築のためネットワーク接続の基礎実験およびヒューマンインターフェイス・立体可視化表現法の基礎技術開発を行なった。分担者として必要な研究情報収集、シミュレーション・コードのモジュール化、および仮想空間における立体可視化の開発に参画した。

(5) 民間企業から奨学寄付金 ～平成17年度 研究代表者、Ca 40,000千円

(6) 所属研究機関(金沢大学)より措置された校費(教育研究費)、研究代表者、Ca. 3,000～5,000千円/年

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