Theoretical Alchemy

Modeling Matter

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Theoretical Alchemy

Modeling Matter

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*To Lucky, and to our delightful and ever-growing
extended family*

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spirit

AUTHOR'S NOTE

IF THIS BOOK HAS A THESIS, IT IS THAT THE BEST WAY TO UNDERSTAND BONDING MAY BE TO TAKE THE APPROPRIATE VIEW FOR EACH MOLECULE OR COMPOUND. A VIEW WHICH MAY BE QUITE DIFFERENT FOR DIFFERENT SYSTEMS. SOMETIMES VERY DIFFERENT VIEWS ARE APPROPRIATE FOR THE SAME SYSTEM, AND A COMBINATION MAY EVEN GIVE THE PARAMETERS NEEDED TO ESTIMATE PROPERTIES SUCH AS COHESION. ONE THEN PROCEEDS BY HAND TO MAKE THE ESTIMATE. THIS OF PROCEEDING CONTRASTS STRONGLY WITH DENSITY FUNCTIONAL THEORY, THE METHOD OF CHOICE FOR MOST SUCH STUDIES INVOLVING SOLIDS. IN THAT ONE SEEKS A SINGLE VIEW, WHICH MAY BE APPLIED TO SYSTEMS, AND THEN APPROACHES IT COMPUTATIONALLY. PERHAPS THAT IS ANOTHER EXAMPLE OF A VIEW ALSO BEING APPROPRIATE.

THE BOOK MIGHT ALSO BE DESCRIBED AS “EVERYTHING YOU NEED TO KNOW IN ORDER TO UNDERSTAND OXIDE FUEL CELLS”, SINCE THAT IS THE CENTER OF MUCH RESEARCH. HOWEVER, THAT UNDERSTANDING REQUIRES AN EXTRAORDINARY BACKGROUND. THE FUEL CELLS SHOW UP PARTICULARLY IN THE LAST SECTION OF THE LAST CHAPTER WHERE OXYGEN ADSORPTION ON MANGANITES IS DISCUSSED. IN COMPARISON IS MADE WITH CURRENT DENSITY-FUNCTIONAL TREATMENT. REGARD, THE BOOK IS AN ARGUMENT FOR A DIFFERENT WAY OF PROCEEDING TO PROBLEMS FROM THE MAINSTREAM APPROACH.

THIS BOOK ALSO CONTRASTS WITH TWO PREVIOUS BOOKS. THE FIRST, *Structure and the Properties of Solids*, APPEARED IN 1989. IN THE MIDST OF

WRITING THAT TEXT A SET OF EMPIRICAL RULES FOR OBTAINING COUPLING BETWEEN NEIGHBORING ATOMIC STATES, SUCH AS THE COUPLING BETWEEN NEIGHBORING s STATES AS $0.42 \hbar^2/md^2$, BECAME A THEORETICAL FINDING $\hbar^2/md^2$. THERE WAS TIME TO REORGANIZE FOR THAT AND I WAS LUCKY ENOUGH TO REDO THE ENTIRE PROGRAM TEN YEARS LATER IN *Electronic Structure*. BOTH TEXTS WERE SOMEWHAT MASSIVE, AND I AM DELIGHTED TO HAVE TEN YEARS LATER TO TRY TO DISTILL THE ESSENCE OF THE REPRESENTATION OF THE STRUCTURE IN A MUCH BRIEFER DESCRIPTION.

THE TWO EARLIER BOOKS WERE WRITTEN AS IF THE READER COULD FIND SOMETHING INTERESTING OR USEFUL WILL BE FOUND. TO BE SURE, THE NEW BOOKS CENTER ON THE INSIGHTS DESCRIBED IN THE EARLIER BOOKS, AND A SERIES OF SUBSEQUENT PAPERS. IT DOES NOT GIVE DUE CREDIT TO THE ESSENTIAL CONTRIBUTIONS OF THE MANY OTHER WORKERS WHO MADE THESE INSIGHTS POSSIBLE, ALL ARE REFERENCED IN THE TWO EARLIER BOOKS. THIS BOOK MIGHT OTHERWISE BE OF A SIMILAR SIZE WHAT REFERENCES THERE ARE, WERE MOSTLY INCLUDED WHERE MORE COMPLETE DESCRIPTIONS EXIST THAN I COULD INCLUDE HERE.

THE BOOK IS ALSO MADE BRIEFER BY FOCUSING PRIMARILY ON THE ENERGIES, THE ENERGY GAINED IN ASSEMBLING A MOLECULE OR A SOLID, OR WITH A SURFACE. A CENTRAL POINT IS THAT THE SAME DESCRIPTION OF THE STRUCTURE WHICH GIVES THE COHESION CAN ALSO BE USED TO UNDERSTAND OTHER PROPERTIES, BUT WE LARGELY LEAVE THAT TO THE OTHER BOOKS. WE HAVE MANY EXTENDED DERIVATIONS TO THE EARLIER TEXTS EXCEPT WHERE THEY ARE PARTICULARLY IN THE EXTENSION TO MOLECULES, AND THEN THEY APPEAR IN THE APPENDICES. HOWEVER, THE SUBJECT IS QUANTITATIVE AND WE USE EQUATIONS AS AN INTEGRAL PART OF THE DISCUSSION.

A NOTE ALSO ON THE TYPOGRAPHY, WHICH MAY LEAVE SOMETHING TO BE DESIRED. I HAVE PREPARED CAMERA-READY COPY USING MICROSOFT WORD. MY INTERESTS OF ECONOMY. ALL SHORTCOMINGS CAN BE ATTRIBUTED TO THE PRESS. TO WORLD SCIENTIFIC PUBLISHING COMPANY. THEY HAVE MY GRATITUDE FOR PROVIDING BOOKS AT REASONABLE PRICES, HARDLY THE CURRENT FASHION. I HOPE THE READER CAN ACCEPT THE RESULT AS SOMETHING BETWEEN A PERSONAL AND A TRADITIONAL BOOK.

ONE PARTICULAR VIEW WHICH HAS PROVEN HELPFUL IS "THEORETICAL CHEMISTRY" IN WHICH WE UNDERSTAND ONE SIMPLE ELEMENT, LIKE THE INERT GAS ARGON. THEN CONCEPTUALLY REMOVE A PROTON FROM THE NUCLEUS OF ONE ARGON ATOM, A CHLORINE NUCLEUS, AND PLACE IT IN THE NUCLEUS OF ANOTHER ARGON ATOM, MAKING IT A POTASSIUM. THE ELECTRON CLOUD WILL SHRINK A LITTLE AROUND THE ARGON AND EXPAND AROUND THE CHLORINE, BUT WE CAN UNDERSTAND THE BEHAVIOR OF THE POTASSIUM CHLORIDE COMPOUND IN TERMS OF THE SIMPLER INERT GAS. I

CENTRAL IDEA OF THIS BOOK, BUT IT COMES UP ENOUGH TO SEEM AN APPROPRIATE TITLE, RATHER THAN SOMETHING LIKE “REINVENTING CHEMISTRY”. WE ALSO DO A COMBINATION OF THE MODERN “THEORY” WITH THE ANCIENT EFFORT OF “ALCHEMISTS” TO MAKE SENSE OF THE MATERIAL WORLD. A GOAL OF THE ORIGINAL ALCHEMICAL TRANSMUTATION OF LEAD TO GOLD, IS THEORETICALLY QUITE EASY; ONE SIMPLY REMOVES THREE PROTONS FROM THE NUCLEUS OF LEAD AND IT IS DONE. WE LEAVE IT TO OUR EXPERIMENTAL COLLEAGUES TO WORK OUT THE DETAILS IN THE LABORATORY.

WAITER A. HARRISON
April, 2010
Stanford, California

Note about the cover: THE PAINTING BY THE AUTHOR, INTENDS TO REPRESENT THE BOOK. THE ALCHEMICAL SYMBOLS BELOW ARE IDENTIFIED AT THE BEGINNING OF EACH CHAPTER. THE RED SYMBOL INSIDE THE FLASK IS FOR OIL OF VITRIOL, THE BILLY GOAT IS AMMONIA; THINK OF IITMUS PAPER. THE CORRESPONDING REACTION IS SHOWN IN THE LOWER PART OF THE PAPER. THERE IS ALSO A FAINT SYMBOL IN THE FLASK FOR THE HYDROGEN BOND IN WATER, FROM CHAPTER 2, AND APPENDIX 2C ON THE NATURE OF THE HYDROGEN BOND. AT THE TOP OF THE PAPER IS AN EQUATION FROM THE STRUCTURE OF SEMICONDUCTORS IN CHAPTER 5. WE HOPE THE BOOK, LIKE THE PAINTING, CAN SHED SOME LIGHT ON A MODERN WAY OF UNDERSTANDING MATTER.

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