

Prof. MURAT ERTÜRK

Personal Information

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International Researcher IDs

ORCID: 0000-0002-7039-1970

Publons / Web Of Science ResearcherID: L-2137-2014

ScopusID: 24461086400

Yoksis Researcher ID: 39953

Education Information

Post Doctorate, Universitaet Stuttgart, Institute for Theoretical Chemistry, Germany 2021 - 2022

Post Doctorate, Nicolaus Copernicus University, Institute of Physics, Poland 2013 - 2014

Doctorate, Canakkale Onsekiz Mart University, Fen Bilimleri Enstitüsü, Fizik, Turkey 2005 - 2011

Postgraduate, Canakkale Onsekiz Mart University, Fen Bilimleri Enstitüsü, Fizik, Turkey 2003 - 2005

Undergraduate, Akdeniz University, Fen-Ed. Fakültesi, Fizik, Turkey 1997 - 2002

Foreign Languages

English, B2 Upper Intermediate

Dissertations

Postgraduate, Bazı çok elektronlu atomların multiplet enerji çiftlenim-izdüşüm katsayılarının hesaplanması , Canakkale Onsekiz Mart University, Fizik, Fizik, 2015

Doctorate, Hartree-fock-roothaan kuramında kesirli baş kuantum sayılı orbitaller kullanılarak atom özelliklerinin incelenmesi, Canakkale Onsekiz Mart University, Fen Bilimleri Enstitüsü, Fizik, 2011

Research Areas

Physics, Atomic and Molecular Physics, Theory of Atoms and Molecules, Atomic and Molecular Interactions, Natural Sciences

Academic Titles / Tasks

Professor, Canakkale Onsekiz Mart University, Fen Fakültesi, Fizik, 2023 - Continues

Associate Professor, Canakkale Onsekiz Mart University, Fen Fakültesi, Fizik, 2019 - 2023

Research Assistant PhD, Canakkale Onsekiz Mart University, Fen Fakültesi, Fizik, 2010 - 2019

Research Assistant, Canakkale Onsekiz Mart University, Lisansüstü Eğitim Enstitüsü, Fizik, 2005 - 2010

Academic and Administrative Experience

Deputy Head of Department, Çanakkale Onsekiz Mart University, Fen Fakültesi, Fizik, 2019 - 2021

Courses

General Physics II, Undergraduate, 2020 - 2021
Advanced Electromagnetic Theory I, Postgraduate, 2020 - 2021
Group Representations II, Doctorate, 2020 - 2021
General Physics II, Undergraduate, 2020 - 2021
General Physics I, Undergraduate, 2018 - 2019, 2017 - 2018
Atom ve Molekül Fiziği , Undergraduate, 2017 - 2018
Fizik, Undergraduate, 2017 - 2018

Advising Theses

Ertürk M., THE APPLICABILITY OF BESSEL TYPE ORBITALS WITH NON-INTEGER PRINCIPAL QUANTUM NUMBERS TO THE CALCULATION OF ELECTRONIC STRUCTURE OF ATOMIC SYSTEMS, Postgraduate, M.COŞKUN(Student), 2020
Ertürk M., Mehmetoğlu B., USE OF COMPLETE SETS OF SELF-FRICTION POLYNOMIALS IN COMBINED HARTREE-FOCK-ROOTHAAN ELECTRONIC STRUCTURE CALCULATIONS, Doctorate, G.DEMİRDAK(Student), 2019

Jury Memberships

Post Graduate, Tez savunma jürisi, Çanakkale Onsekiz Mart Üniv. FBE Fizik Anabilim Dalı, September, 2017

Published journal articles indexed by SCI, SSCI, and AHCI

- I. Generalized Complete Orthonormal Sets of Exponential-Type Functions (Chem. Phys.)
Demirdak G., Şahin E., Ertürk M.
CHEMICAL PHYSICS, vol.570, no.111893, pp.1-5, 2023 (SCI-Expanded)
- II. Applicability of Noninteger Bessel Type Orbital Basis Sets: Numerical and Analytical Approaches
Coşkun M., Ertürk M.
JOURNAL OF MATHEMATICAL CHEMISTRY, vol.61, no.0, pp.1672-1683, 2023 (SCI-Expanded)
- III. Exponential type orbitals with hyperbolic cosine function basis sets for isoelectronic series of the atoms Be to Ne
Şahin E., ERTÜRK M., Ozdogan T., Orbay M.
Zeitschrift fur Naturforschung - Section A Journal of Physical Sciences, vol.78, no.1, pp.1-8, 2023 (SCI-Expanded)
- IV. Comparative performance of different hyperbolic cosine functions and generalized B functions basis sets for atomic systems
Ertürk M., Coşkun M.
PHYSICA SCRIPTA, vol.97, no.7, pp.1-11, 2022 (SCI-Expanded)
- V. Double hyperbolic cosine basis sets for LCAO calculations
Coskun M., Ertürk M.
MOLECULAR PHYSICS, vol.120, no.17, 2022 (SCI-Expanded)
- VI. Generalized B functions applied to atomic calculations
ERTÜRK M., Şahin E.
CHEMICAL PHYSICS, vol.529, 2020 (SCI-Expanded)
- VII. Modified B function basis sets with generalized hyperbolic cosine functions
Erturk M., Ozturk E.

- COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1127, pp.37-43, 2018 (SCI-Expanded)
- VIII. **Size-Extensivity Corrections in Single- and Multireference Configuration Interaction Calculations**
ERTÜRK M., Meissner L.
ELECTRON CORRELATION IN MOLECULES - AB INITIO BEYOND GAUSSIAN QUANTUM CHEMISTRY, vol.73, pp.145-160, 2016 (SCI-Expanded)
- IX. **A posteriori corrections to the configuration interaction method: a single-reference and multi-reference study**
Erturk M., Meissner L.
MOLECULAR PHYSICS, vol.113, pp.3014-3022, 2015 (SCI-Expanded)
- X. **Exponential type orbitals with generalized hyperbolic cosine functions for atomic systems**
Erturk M.
COMPUTER PHYSICS COMMUNICATIONS, vol.194, pp.59-63, 2015 (SCI-Expanded)
- XI. **An improvement on psi((alpha)*())-exponential type orbitals for atoms in standard convention**
Guseinov I. I., ŞAHİN E., ERTÜRK M.
MOLECULAR PHYSICS, vol.112, no.1, pp.35-40, 2014 (SCI-Expanded)
- XII. **An Improvement on Noninteger n-Generalized Exponential Type Orbitals with Hyperbolic Cosine in Atomic Calculations**
Erturk M.
BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN, vol.85, no.7, pp.753-757, 2012 (SCI-Expanded)
- XIII. **Use of noninteger n-generalized exponential type orbitals with hyperbolic cosine in atomic calculations**
Guseinov I. I., Erturk M.
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.112, no.6, pp.1559-1565, 2012 (SCI-Expanded)
- XIV. **Use of combined Hartree-Fock-Roothaan theory in evaluation of lowest states of K[Ar]4s03d1 and Cr+[Ar]4s 03d5 isoelectronic series over noninteger n-Slater type orbitals**
Guseinov I. I., Erturk M., Sahin E.
Pramana - Journal of Physics, vol.76, no.1, pp.109-117, 2011 (SCI-Expanded)
- XV. **Application of Combined Hartree-Fock-Roothaan Theory to Isoelectronic Series of Atoms Using Noninteger n-Generalized Exponential Type Orbitals**
Guseinov I. I., Erturk M.
MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY, vol.61, no.3, pp.603-613, 2009 (SCI-Expanded)
- XVI. **Use of noninteger n-Slater type orbitals in combined Hartree-Fock-Roothaan theory for calculation of isoelectronic series of atoms Be to Ne**
Guseinov I. I., Ertuerk M.
International Journal of Quantum Chemistry, vol.109, no.2, pp.176-184, 2009 (SCI-Expanded)
- XVII. **Construction of different kinds of atomic and molecular orbitals using complete orthonormal sets of $\Psi\alpha$ -ETO in single exponent approximation**
Israfil G. I., Murat E.
Chinese Physics Letters, vol.25, no.7, pp.2444-2447, 2008 (SCI-Expanded)
- XVIII. **Calculation of negative ions of B, C, N, O and F using noninteger n Slater type orbitals**
Guseinov I. I., Ertuerk M., ŞAHİN E., Aksu H., Bagci A.
Journal of the Chinese Chemical Society, vol.55, no.2, pp.303-306, 2008 (SCI-Expanded)
- XIX. **Calculations of isoelectronic series of He using noninteger n-Slater type orbitals in single and double zeta approximations**
Guseinov israfil G. i., Ertoerk Murat E. M., Sahin Ercan S. E., Aksu Hueseyin A. H.
Chinese Journal of Chemistry, vol.26, no.1, pp.213-215, 2008 (SCI-Expanded)
- XX. **Application of combined Hartree-Fock-Roothaan theory to atoms with an arbitrary number of closed and open shells of any symmetry**
GUSEINOV I. I., Mamedov B. A., Ertuerk M., AKSU H., ŞAHİN E.
FEW-BODY SYSTEMS, vol.41, pp.211-220, 2007 (SCI-Expanded)

Articles Published in Other Journals

I. Noninteger Bessel Type Orbitals for Two Electron Atomic Systems

COŞKUN M., Ertürk m.

Journal of advanced research in natural and applied sciences (Online), vol.9, no.2, pp.375-384, 2023 (Peer-Reviewed Journal)

Refereed Congress / Symposium Publications in Proceedings

I. COMPUTATION OF THERMOCHEMICAL PROPERTIES BASED ON INTERNALLY CONTRACTED MULTIREFERENCE COUPLED-CLUSTED METHODS

Ertürk M., Köhn A.

6th International Conference on Molecular Electronic Structure, (MES), Monastir, Tunisia, 2 - 06 September 2022, pp.15

II. APPLICABILITY AND EFFECTIVENESS OF BESSEL TYPE ORBITALS WITH NONINTEGRAL ORDERS TO CALCULATION OF ISOELECTRONIC SERIES OF HE ATOM

Ertürk M., Coşkun M.

TÜRK FİZİK DERNEĞİ 38. ULUSLARARASI FİZİK KONGRESİ, Muğla, Turkey, 31 August - 04 September 2022, pp.79

III. The Applicability of Bessel Type Orbitals With Non-Integer Principal Quantum Numbers to The Calculation of Electronic Structure of Atomic Systems

Ertürk M., Coşkun M.

2 ND INTERNATIONAL CONFERENCE ON APPLIED ENGINEERING AND NATURAL SCIENCES, Konya, Turkey, 10 - 13 March 2022, pp.1

IV. Size-extensive Corrected Configuration interaction potential energy curves for the ground and excited states of some diatomic molecules

Ertürk M.

Türk Fizik Derneği 37. Uluslararası Fizik Kongresi, Muğla, Turkey, 1 - 05 September 2021, pp.84

V. Understanding of the Quantum Nature of Electron Transfer and Explaining Spectral Asymmetries in Photosynthetic Bacteria Reaction Center: Screened Range-Separated Density Functional Theory

Ertürk M., Aksu H., Demirdak G., D. Dunietz B.

Virtual Molecular Electronic Structure Conference, Warszawa, Poland, 1 - 04 September 2020, pp.1

VI. Towards more Precise and Flexible Basis Function in SCF Calculations: Generalizing Complete Orthonormal Sets of Exponential Type Orbitals

Ertürk M., Demirdak G.

Türk Fizik Derneği 35. Uluslararası Fizik Kongresi, Muğla, Turkey, 4 - 08 September 2019, pp.1

VII. Unrestricted B functions for LCAO Calculations

Coşkun M., ERTÜRK M., ŞAHİN E.

TFD 34. Uluslararası Fizik Kongresi, Muğla, Turkey, 5 - 09 September 2018

VIII. Effect of Noniterative Connected Triples in the Coupled-Cluster Corrections: Single Reference Calculations

ERTÜRK M.

Türk Fizik Derneği 33. Uluslararası Fizik Kongresi, 6 - 10 September 2017

IX. Improving the Performance of Bessel Type Orbitals

ERTÜRK M., Öztürk E.

Türk Fizik Derneği 33. Uluslararası Fizik Kongresi, 6 - 10 September 2017

X. Konfigürasyon etkileşim yöntemindeki size-extensivity problemine yapılan coupled-cluster düzeltme yaklaşımındaki gelişmeler

ERTÜRK M.

ADIM FİZİK GÜNLERİ VI, Turkey, 19 - 21 July 2017

XI. THE PERFORMANCE OF THE VARIOUS SIZE EXTENSIVITY CORRECTION METHODS IN

- MULTIREFERENCE CI APPROACH A COMPARATIVE STUDY OF EXCITED STATES OF MOLECULES**
ERTÜRK M.
- TÜRK FİZİK DERNEĞİ 32.ULUSLARARASI FİZİK KONGRESİ, 6 - 09 September 2016**
- XII. Alternatif üstel tipli orbitaller hiperbolik kosinüs tiplifonksiyonlarının verimliliği**
ERTÜRK M., ÖZDER S., Öztürk E.
ADIM FİZİK GÜNLERİ V, Eskişehir, Turkey, 21 - 23 April 2016
- XIII. Yeni tam ortonormal üstel tipli fonksiyonların Hartree Fock yaklaşımında etkin kullanımı**
ERTÜRK M., Aksoy S.
ADIM FİZİK GÜNLERİ V, Eskişehir, Turkey, 21 - 23 April 2016
- XIV. Konfigürasyon etkileşimi yöntemlerine yapılan a posteriori düzeltme yaklaşımları moleküllerin uyarılmış durumları için karşılaştırma**
ERTÜRK M.
ADIM FİZİK GÜNLERİ V, Eskişehir, Turkey, 21 - 23 April 2016
- XV. Bazı Açık Kabuklu Atomlar İçin Hartree Fock Roothaan Denklemlerinin STO Bazında Çözülmesi**
I I G., MEHMETOĞLU B., ERTÜRK M., Aksu H.
Atom-Molekül ve Çekirdek Sistemlerinin Yapıları ve Spektrumları Çalıştayı, Çanakkale, Turkey, 8 - 10 July 2005,
pp.32-37
- XVI. APPLICATION OF THE SIZE EXTENSIVITY CORRECTIONS APPROACHES TO THE LIMITED CONFIGURATION INTERACTION METHODS**
Bozdoğan E., Kuş E., ERTÜRK M.
9th International Physics Conference of the Balkan Physical Union, İstanbul, Turkey, 24 - 27 August 2015
- XVII. USE OF DIAGRAMMATIC TECHNIQUES IN COUPLED CLUSTER THEORY**
Bozdoğan E., Kuş E., ERTÜRK M.
9th International Physics Conference of the Balkan Physical Union, İstanbul, Turkey, 24 - 27 August 2015
- XVIII. Elektron korelasyon yöntemlerinde iki matematiksel formalizmin karşılaştırılması**
Öztürk E., ERTÜRK M.
ADIM Fizik Günleri IV, Kütahya, Turkey, 28 - 29 May 2015
- XIX. ATOMLARIN TEMEL DURUM ENERJİSİNİN HESAPLANMASINDA GENELLEŞTİRİLMİŞ KOSİNÜS HİPERBOLİK FONKSİYONLARININ KULLANILMASI**
Öztürk E., ERTÜRK M.
ADIM Fizik Günleri IV, Kütahya, Turkey, 28 - 29 May 2015
- XX. TEK VE ÇOK REFERANSLI KONFIGÜRASYON ETKILEŞMESİ YÖNTEMİNDE KULLANILAN BAZI SIZE EXTENSIVITY DÜZELTME YÖNTEMLERİNİN KARŞILAŞTIRILMASI**
Öztürk E., ERTÜRK M.
ADIM Fizik Günleri IV, Kütahya, Turkey, 28 - 29 May 2015
- XXI. Comparison of Size extensivity Corrections in Single and Multi Reference Configuration Interaction Methods Ground and Excited States**
ERTÜRK M.
Molecular Electronic Structure Workshop - 2014 (MES 2014), Amasya, Turkey, 1 - 05 September 2014
- XXII. Hyperbolic Cosine and Generalized Hyperbolic Cosine Functions with Exponential Type Orbitals**
Aksoy S., ERTÜRK M.
Molecular Electronic Structure Workshop - 2014 (MES 2014), Amasya, Turkey, 1 - 05 September 2014
- XXIII. On the accuracy of atomic calculations using exponential type orbitals with modified hyperbolic cosine functions**
Aksoy S., ERTÜRK M.
Türk Fizik Derneği 29. Uluslararası Fizik Kongresi, Bodrum, Turkey, 5 - 08 September 2012
- XXIV. Calculations of ground state total energies for atoms using exponential type functions with hyperbolic cosine functions**
Fırat S., ERTÜRK M.
Türk Fizik Derneği 29. Uluslararası Fizik Kongresi, Bodrum, Turkey, 5 - 08 September 2012
- XXV. A Comparative Study of Two Kinds of Hyperbolic Cosine Functions with Exponential Type Functions**

- for Atomic Calculations**
ERTÜRK M.
 Chemical Physics Congress-IX, İzmir, Turkey, 14 - 16 October 2010
- XXVI. Use of Noninteger N Slater TYPE Functions With Generalized Hyperbolic Cosine Functions for Atomic Calculations**
ERTÜRK M.
 Türk Fizik Derneği 27. Uluslararası Fizik Kongresi, İstanbul, Turkey, 14 - 17 September 2010
- XXVII. COMPARISON OF MØLLER PLESSET PERTURBATION AND CONFIGURATION INTERACTION WITH SINGLE AND DOUBLE CALCULATIONS FOR BE AND NE USING SLATER TYPE BASIS SETS**
ERTÜRK M.
 Türk Fizik Derneği 26. Uluslararası Fizik Kongresi, Bodrum, Turkey, 24 - 27 September 2009
- XXVIII. Calculations of isoelectronic series of some open shell atoms using generalized exponential functions**
ERTÜRK M., I I G.
 Türk Fizik Derneği 25. Uluslararası Fizik Kongresi, Bodrum, Turkey, 25 - 29 August 2008
- XXIX. NONINTEGER n STOs and GENERALIZED EXPONENTIAL FUNCTIONS APPLIED TO COMBINED HARTREE FOCK ROOHAAN CALCULATIONS FOR OPEN SHELL ATOMS**
ERTÜRK M., I I G.
 8. KİMYASAL FİZİK KONGRESİ, İstanbul, Turkey, 24 - 25 April 2008
- XXX. Use of noninteger n Slater type orbitals in calculation of isoelectronic series of the atoms Be to Ne**
ERTÜRK M., Israfil I G.
 Symposium on Advanced Methods of Quantum Chemistry and Physics SAMQCP 2007, Torun, Poland, 2 - 06 September 2007
- XXXI. Application of Hartree Fock Roothaan Theory to Atoms and Molecules with Arbitrary Number of Open Shells**
 Guseinov I. I., MEHMETOĞLU B., Bağcı A., Şahin E., ERTÜRK M., Aksu H., Özcan N.
 Türk Fizik Derneği 24. Uluslararası Fizik Kongresi, Malatya, Turkey, 28 - 31 August 2007
- XXXII. Use of complete orthonormal sets of exponential type orbitals in Hartree Fock Roothaan theory**
Israfil I G., MEHMETOĞLU B., ERTÜRK M., Aksu H., Şahin E.
 6th International Conference of the Balkan Physical Union, İstanbul, Turkey, 22 - 26 August 2006
- XXXIII. Bazı Hafif Atomların Multiplet Terim Enerjilerinin ETO Bazları kullanılarak Hesaplanması**
 Israfil H., ERTÜRK M., Aksu H.
 2005 Dünya Fizik Yılı Türk Fizik Derneği 23. Uluslararası Fizik Kongresi, Muğla, Turkey, 13 - 16 September 2005
- XXXIV. Bazı açık kabuklu atomlar ve iyonlar için Hartree-Fock-Roothaan denklemlerinin STO bazında çözümlesi**
 Guseinov I. I., Mehmetoğlu B., Ertürk M., Aksu H.
 Atom-Molekül ve Çekirdek Sistemlerinin Yapıları ve Spektrumları, Çanakkale, Turkey, 8 - 10 July 2005, pp.32-37
- XXXV. Bazı Hafif Atomlar İçin Hartree Fock Roothaan Yöntemi İle Multiplet Terim Enerjilerinin Hesaplanması**
I I G., Yazıcı E., Şahin E., ERTÜRK M.
 Türk Fizik Derneği 22. Fizik Kongresi, Bodrum, Turkey, 14 - 17 September 2004

Supported Projects

HÜSEYİN İ., ERTÜRK M., Project Supported by Higher Education Institutions, HARTREE-FOCK-ROOTHAN KURAMINDA KESİRLİ BAŞ KUANTUM SAYILI ORBITALLER KULLANILARAK ATOM ÖZELLİKLERİİNİN İNCELENMESİ, 2007 - Continues
 Ertürk M., Aksu H., Dunietz B., TUBITAK Project, Ab initio Elektronik Yapı Yöntemleri ile Fotosentetik Işık Hasat Sistemlerinde Enerji ve Yük Transfer Mekanizmalarının İncelenmesi, 2023 - 2025

Ertürk M., Coşkun M., Project Supported by Higher Education Institutions, Çoklu Referans Eşleşmiş Grup Yöntemleri ile Termokimyasal Özelliklerin Hesaplanması, 2023 - 2024

ERTÜRK M., Coşkun M., BAĞCI A., Project Supported by Higher Education Institutions, ATOMİK VE MOLEKÜLER ENERJİ HESAPLAMALARI İÇİN GENELLEŞTİRİLMİŞ ATOMİK ÜSTEL BAZ FONKSİYONLARI VE UYGULAMALARI, 2022 - 2023

ERTÜRK M., Demirdak G., ŞAHİN E., Project Supported by Higher Education Institutions, GENELLEŞTİRİLMİŞ TAM ORTONORMAL FONKSİYONLAR İLE BAZI ATOMİK ORBİTALLERİN OPTİMİZE EDİLMİŞ PARAMETRELERİNİN ELDE EDİLMESİ, 2019 - 2021

ERTÜRK M., COŞKUN M., Project Supported by Higher Education Institutions, BAŞ KUANTUM SAYISI TAM SAYI OLMAYAN BESSEL TİPLİ ORBİTALLERİN ATOMİK SİSTEMLERİN ELEKTRONİK YAPI HESAPLAMALARINA UYGULANABİLİRLİĞİ, 2019 - 2020

Ertürk M., Özdoğan T., Orbay M., Şahin E., Project Supported by Higher Education Institutions, Be-Ne arası atomların izoelektronik serilerinin hiperbolik kosinüs fonksiyonu içeren üstel tipli orbitaller kullanılarak incelenmesi, 2017 - 2019

ERTÜRK M., ŞAHİN E., Project Supported by Higher Education Institutions, ALTERNATİF ÜSTEL TİPLİ ORBİTALLERİN ATOMLARIN TEMEL DURUM ENERJİ HESAPLAMALARINDA KULLANILABİLİRLİĞİNİN İNCELENMESİ, 2017 - 2018

Demircan O., Özdemir S., Ertürk M., TUBITAK Project, Atomlara Ait Multiplet Tablolarının Kuantum Mekaniksel yolla Yenilenmesi, 2004 - 2007

Scientific Refereeing

CMES-COMPUTER MODELING IN ENGINEERING, SCI Journal, March 2022

TURKISH JOURNAL OF CHEMISTRY, SCI Journal, July 2021

Turkish Journal of Chemistry, SCI Journal, March 2019

Journal of Scientific Perspectives, Other Indexed Journal, February 2019

Turkish journal of physics, Other Indexed Journal, August 2016

International Journal of Quantum chemistry, SCI Journal, January 2016

Computer Physics Communications, SCI Journal, January 2015

Metrics

Publication: 60

Citation (WoS): 89

Citation (Scopus): 102

H-Index (WoS): 6

H-Index (Scopus): 6

Congress and Symposium Activities

Molecular Electronic Structure Workshop - 2014, Invited Speaker, Amasya, Turkey, 2014

Scholarships

Computation of Thermochemical Data, TUBITAK, 2021 - 2022

Advanced ab initio methods for describing ground and excited states in atomic and molecular systems, TUBITAK, 2013 - 2014

Awards

ERTÜRK M., poster ödülü: Hyperbolic Cosine and Generalized Hyperbolic Cosine Functions with Exponential Type Orbitals, Molecular Electronic Structure Workshop - 2014 (MES 2014), September 2014

ERTÜRK M., Poster Ödülü: Comparative study of Hyperbolic Cosine Functions with Generalized Exponential Functions and Slater Type Functions for the Ground States of Atoms, International Workshop on QUANTUM SYSTEMS IN CHEMISTRY, PHYSICS, August 2010